REMEDIAL GOAL OPTION REPORT
FOR
THE DEVELOPMENT OF PRELIMINARY REMEDIATION GOALS IN SEDIMENT AND FLOODPLAIN SOILS, REVISION 3

OPERABLE UNIT 2, McINTOSH, ALABAMA

Prepared for:

OLIN CORPORATION

Cleveland, Tennessee

Prepared by:

3200 Town Point Drive NW, Suite 100
Kennesaw, Georgia 30144

July 6, 2012

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Project No. 6107-12-0036

EPA Preface

This preface presents the EPA perspective on the Remedial Goal Option Report for Olin McIntosh OU-2, Revised July 6, 2012. Though uncertainty remains in some areas, EPA believes that the results of the human health and ecological risk assessments adequately allow for the development of preliminary remedial goals (PRGs) for mercury, DDTR, and HCB.

Olin calculated PRGs for mercury in sediment and soil using two different methodologies. The first methodology used site-specific tissue and sediment data to define bioaccumulation relationships (BSAFs or BAFs) for mercury and DDTR in sediment and soil moving through the food chain into prey items utilized by the ecological receptors. This methodology involves establishing a correlation between sediment and tissue concentrations, or deriving a simple ratio between tissue and sediment concentrations depending upon the available data. The resulting relationship is then used to identify the sediment/soil concentrations that result in a tissue concentration that triggers a risk to the receptor feeding on that tissue. The sediment or soil concentration that results in a tissue concentration that triggers risk (i.e. results in a dose exceeding the NOAEL toxicity reference value) to an upper-trophic level receptor is then identified as the PRG for that receptor. This is the traditional way that PRGs are derived for most contaminants based on food chain modeling results. The second methodology Olin used to derive PRGs was the Spreadsheet Ecological Risk Assessment For Mercury (SERAFM) model, which was developed by EPA ORD. EPA recommended that Olin develop PRGs using both methodologies, and that the results from both would be considered in a weight of evidence approach to select clean-up goals from the range of PRGs developed.

In establishing BSAF or BAF relationships, EPA directed that only regression relationships with a correlation coefficient >0.70 should be considered, and that data sets with a correlation coefficient <0.70 should default to a simple ratio method to define the bioaccumulation relationship. EPA also recommended that the geometric mean between the NOAEL and LOAEL be used as the preferred risk level for PRG derivation.

One of the main sources of uncertainty in the derivation of PRGs using the BAFs, BSAF, and ratio methods is how data are paired spatially and temporally. Sediment and fish data sets in OU-2 span a number of years, and biota such as fish move around, therefore they do not get their exposure from any one location. Data must be averaged across appropriate spatial scales for the exposed organism.

As mentioned in the preface to the ecological and human health risk assessments, uncertainty exists in the evaluation of belted kingfisher risk and the subsequent derivation of Toxicity Reference Values (TRVs) due to differences in preferred exposure parameters between Olin and EPA. The lowest BSAF-based PRGs for mercury and DDTR in sediment are both based on protection of belted kingfisher using the EPA-preferred exposure model. Mercury PRGs for all modeled species that have fish as part of their diet are shown in Table F-3. DDTR BAF/BSAF-derived PRGs

for all modeled species that have fish as part of their diet are shown in Table F-4. As previously noted, EPA agreed to consider the entire range of PRGs for piscivorous receptors when choosing clean-up goals.

Table F-3. BAF/BSAF-derived Mercury PRGs For Piscivorous Birds in Olin OU-2

Receptor	Whole Body Forage Fish Mercury Concentration That Triggers Risk	Sediment PRG Based on Geometric Mean of NOAEL and LOAEL
Belted Kingfisher (EPA Model)	0.11 mg/kg	0.36 mg/kg
Little Blue Heron	0.20 mg/kg	1.6 mg/kg
Belted Kingfisher (Olin Model)	0.35 mg/kg	6.5 mg/kg
Pied-billed Grebe	0.58 mg/kg	25 mg/kg
	Whole Body Predatory Fish Concentration That Triggers Risk	Sediment PRG Based on Geometric Mean of NOAEL and LOAEL
Great Blue Heron	0.43 mg/kg	1.7 mg/kg

Table F-4. BAF/BSAF-derived DDTR PRGs For Piscivorous Birds in Olin OU-2

Receptor	Whole Body Forage Fish DDTR Concentration That Triggers Risk	Sediment PRG Based on Geometric Mean of NOAEL and LOAEL
Belted Kingfisher (EPA Model)	0.47 mg/kg	0.33 mg/kg
Little Blue Heron	0.71mg/kg	0.58 mg/kg
Belted Kingfisher (Olin Model)	0.98 mg/kg	0.91 mg/kg
Pied-billed Grebe	0.78 mg/kg	0.66 mg/kg
Great Blue Heron	1.52 mg/kg	1.7 mg/kg

Derivation of PRGs using the same receptors in the SERAFM model yields higher PRGs than using the BAF/BSAF approach. Many aspects of the SERAFM model are customizable to use site-specific information and data. EPA and Olin held extensive discussions on appropriate data and parameters to use to make the model site specific, and reached agreement on those data and parameters prior to finalization of model results. One potential explanation for why the SERAFM model yielded higher PRGs is that the SERAFM model treats mercury bioaccumulation as a linear function, while the BSAF approach used a power curve function to define mercury bioaccumulation into fish. In the power curve, mercury bioaccumulations rates are higher at lower levels of mercury in sediment, and level off as mercury in sediment increases. The explanation for why mercury in sediment may not bioaccumulate in a linear fashion is that mercury bioaccumulation in aquatic systems is primarily a function of methylmercury production, and at higher levels of mercury in sediment, the amount of total mercury available is no longer the limiting factor in methylmercuy production. EPA will consider the range of PRGs derived from the

different methodologies, and for the full range of receptors in selecting clean-up goals for mercury and DDTR. The recommended risk-based PRGs expected to provide protection of ecological receptors, and the basis for their selection, is shown in Table F-5. It is important to note that risk-based PRGs for DDTR in sediment and flood plain soil are less than upgradient concentrations of DDTR at the BASF site. The concentrations of DDTR in sediment protective of piscivorous birds at the Olin McIntosh site are lower than those at the BASF (Ciba) site due to differences in habitat and species composition between the two areas. The Olin site has permanent ponded water that allows larger fish to be present that bioaccumulate more DDTR than the mosquito fish in ephemeral ponds at the Ciba site. Whether or not risk-based PRGs at Olin OU-2 can be achieved while potential upgradient sources remain in place is a risk management decision that will be addressed in the Record of Decision.

Table F-5. Recommended Risk-based PRGs for Mercury, HCB, and DDTR

Habitat Type/ Name	Exposure Medium	COC	Protective Level	Units	Basis	Assessment Endpoint
	Sediment	Mercury	1.6 to 10.7	mg/kg	Lower end of range based on geometric mean of NOAEL and LOAEL PRGs for little blue heron derived using sediment to fish BSAF uptake model. Upper end of range based on NOAEL PRG derived from SERAFM mercury uptake model for little blue heron.	Protection of piscivorous birds (little blue heron)
		HCB	7.6	mg/kg	NOAEL	Protection of piscivorous mammals (mink)
		DDTR	0.58 to 1.7	mg/kg	Lower end of range based on geometric mean of NOAEL and LOAEL PRGs for little blue heron. Upper end of range based on geometric mean of NOAEL and LOAEL PRGs for great blue heron.	Protection of piscivorous birds (little blue heron and great blue heron)
	Floodplain Soil	Mercury	1.7	mg/kg	NOAEL PRG based on ingestion of crawling insects and spiders	Protection of terrestrial insectivorous birds
		DDTR	0.14	mg.kg	Geometric mean of NOAEL and LOAEL PRGs for Carolina wren feeding on crawling insects and spiders	Protection of terrestrial insectivorous birds

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LIST OF ACRONYMS AND ABBREVIATIONS

Acronym	Definition
95UCL	95 percent upper confidence limit
AMEC	AMEC Environment & Infrastructure, Inc.
AOC	Administrative Order of Consent
AWQC	ambient water quality criterion
BAF	bioaccumulation factor
Basin	Olin Basin
BSAF	biota-sediment accumulation factor
CFR	Code of Federal Regulations
COC	constituent of concern
CT	central tendency
DDD	Dichlorodiphenyldichloroethane
DDE	Dichlorodiphenyldichloroethylene
DDT	Dichlorodiphenyltrichloroethane
DDTR	2,4'- and 4,4'-isomers of DDD, DDE, and DDT
dw	Dry Weight
EPC	exposure point concentration
ERA	ecological risk assessment
ESPP	enhanced sedimentation pilot project
FOC	fraction of organic carbon
FS	Feasibility Study
g/m^3	gram per cubic meter
HCB	Hexachlorobenzene
HI	Hazard Index
HRT	hydraulic residence time
LOAEL	lowest observed adverse effect level
µg/L	microgram per liter
mg/kg	milligram per kilogram
NAVD88	North American Vertical Datum of 1988
NCP	National Oil and Hazardous Substances Pollution Contingency Plan
Neptune	Neptune and Company, Inc.

Acronym	Definition
NOAEL	no observed adverse effect level
NPDES	National Pollutant Discharge Elimination System
Olin	Olin Corporation
OU-1	Operable Unit 1
OU-2	Operable Unit 2
PRG	preliminary remediation goal
R^2	coefficient of determination
RCRA	Resource Conservation and Recovery Act
RGO	remedial goal option
RI	Remedial Investigation
RME	reasonable maximum exposure
river	Tombigbee River
SERAFM	spreadsheet-based ecological risk assessment for the fate of mercury
site	McIntosh, Washington County, Alabama Plant Site
TRV	toxicity reference value
URS	URS Corporation
USEPA	U.S. Environmental Protection Agency
WCC	Woodward-Clyde Consultants
ww	wet weight

1.0 INTRODUCTION

Olin Corporation (Olin) has prepared Remedial Investigation/Feasibility Study (RI/FS) Reports for its McIntosh, Washington County, Alabama, Plant Site (site) under the oversight of the U.S. Environmental Protection Agency (USEPA). The site is an active chemical production facility, located approximately 1 mile east-southeast of the town of McIntosh, Washington County, Alabama (Figure 1-1). The site is listed on the National Priority List of the Comprehensive Environmental Response, Compensation, and Liability Act. Olin signed an Administrative Order of Consent, effective May 9, 1990, to satisfy the National Oil and Hazardous Substances Pollution Contingency Plan (NCP) (40 Code of Federal Regulations [CFR] 300). The site consists of two operable units. Operable Unit 1 (OU-1) comprises the Olin property, except Operable Unit 2 (OU-2), and includes the manufacturing process areas. OU-2 comprises the Olin Basin (Basin), Round Pond, surrounding wetlands on the Olin property, and the former wastewater ditch that discharged from the Basin from 1952 to 1974 (Figure 1-1).

Numerous studies have been conducted at the site. The FS and implementation of the remedial action have been completed for OU-1 and are being monitored under the Resource Conservation and Recovery Act (RCRA). The revised RI Addendum and FS for OU-2 were submitted to USEPA in November 14, 2011 and April 9, 2012, respectively.

1.1 SITE DESCRIPTION AND BACKGROUND

The Basin and Round Pond comprise approximately 76 and 4 acres, respectively. The Basin is located between a bluff to the west and the Tombigbee River (river) to the east. The bluff is approximately 20 to 30 feet higher in elevation than the floodplain area near the Basin. The Basin and Round Pond are thought to be part of a former natural oxbow lying within the floodplain of the river. The wastewater ditch extends from OU-1 to the inlet channel.

The primary constituent of concern (COC) at OU-2 is mercury, which best represents the extent of contamination in sediments and biota in the Basin and Round Pond. USEPA has also requested the evaluation of other COCs, including hexachlorobenzene (HCB) and the 2,4′- and 4,4′-isomers of dichlorodiphenyltrichloroethane (DDT), dichlorodiphenyldichloroethylene (DDE), and dichlorodiphenyl-dichloroethane (DDD) (collectively, DDTR). The primary release mechanism for mercury and HCB to OU-2 was the discharge through the former wastewater ditch (Figure 1-1) from 1952 to 1974 (Woodward-Clyde Consultants [WCC], 1993). Surface runoff and treated wastewater from the Plant were

not discharged to the Basin after 1974. The plant effluent and stormwater discharge are permitted and monitored under the National Pollutant Discharge Elimination System (NPDES). The current discharge is acceptable within NPDES limits. Manufacturing activities at the Olin McIntosh Plant have not included DDTR.

The primary release mechanism for DDTR is migration of sediments and soils containing DDTR from the BASF property (formerly Ciba-Geigy), located north of OU-2, where DDT was manufactured during the same timeframe as the mercury and HCB discharge. DDTR concentrations have historically been highest in the northern portion of OU-2 along the Olin-BASF property line.

The Basin is enclosed by the enhanced sedimentation pilot project (ESPP). The ESPP includes a berm and gate system and an inlet channel that provides hydraulic connection between the Basin and the river. The primary purpose of this constructed system is to enhance the capture of sediment-laden floodwaters in the Basin and then hold the water and sediment to allow the sediment to be deposited within the Basin. A secondary purpose of the berm and gate system is to control water levels to reduce wind-driven resuspension of sediments.

1.2 PURPOSE

The purpose of this remedial goal option (RGO) document is to present preliminary remediation goals (PRGs) that have been developed for mercury, HCB, and DDTR in sediment and floodplain soils.

1.3 STATUS

This RGO document is a supplement to two other documents, which have been approved by USEPA:

- *Part 1: Remedial Investigation Addendum and Enhanced Sedimentation Pilot Project Annual Report—Year Two Results* (AMEC Environment & Infrastructure, Inc. [AMEC], 2011a)
- *Part 2: Updated Ecological Risk Assessment* (ERA) (AMEC, 2011b)

These documents were submitted to USEPA on November 14, 2011, and included summaries of historical and current data, including surface water and sediment data collected in 2006, 2008, and 2009. These documents also include results of floodplain, insect, and vegetation samples collected in June 2010.

1.4 PRG CALCULATION METHODS

PRGs for sediment were calculated using four methods:

- **Biota-sediment Accumulation Factor (BSAF).** PRGs for mercury and DDTR were calculated using the BSAF method. The BSAF method is a four-step process. Average fish tissue concentrations were first graphed against average sediment concentrations based on the home ranges of various fish species. Site-specific regression equations relating the tissue concentrations to sediment concentrations were then developed using the graphs. The target fish tissue concentration was then determined by back calculation of the aquatic risk equations presented in the updated ERA (AMEC, 2011b). The target fish tissue concentration was entered into the site-specific regression equation to obtain a corresponding target sediment concentration (PRG). The results of this analysis are presented in Section 2.0.

- **The Ratio Method.** PRGs for mercury and DDTR were calculated by dividing the average fish tissue concentration by the average sediment concentration. Home ranges of the various fish species were not considered in the ratio method. This approach is a simplified description of bioaccumulation and assumes mercury and DDTR concentrations in fish increase without an upper bound as sediment concentrations increase. Results are presented in Section 2.0.

- **Direct Calculation of PRG.** The PRG for HCB was estimated by direct reduction of sediment concentration in the forward risk calculation to achieve a hazard index (HI) equivalent to 1. The BSAF approach was not required for HCB since risk was driven by direct ingestion of abiotic media (i.e., sediment) and not through ingestion of prey items that may bioaccumulate HCB through the food chain. Results are presented in Section 2.0.

- **Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury (SERAFM).** SERAFM is a Microsoft® Excel model provided by USEPA that is used to estimate target mercury sediment concentrations for aquatic ecological receptors. Detailed discussion of the scenarios modeled under SERAFM and results are presented in Section 3.0.

PRGs for floodplain soils were calculated using the following method:

- **Soil-to-invertebrate Bioaccumulation Factor (BAF).** Invertebrate tissue concentrations were graphed against average floodplain soil concentrations (0- to 6-inch-depth interval), and site-specific regression equations relating the tissue concentrations to surface soil concentrations were developed. The target invertebrate tissue concentration was then determined by back calculation of the terrestrial risk equations presented in the updated ERA (AMEC, 2011b). The target invertebrate tissue concentration was entered into the site-specific regression equation to obtain a corresponding target surface soil concentration (PRG). Detailed discussion of this method for PRG calculation is presented in Section 4.0.

- **The Ratio Method.** PRGs for mercury and DDTR were calculated by dividing the average invertebrate tissue concentration by the average floodplain soil concentration. Home ranges of the various invertebrate species were not considered in the ratio method. This approach is a simplified description of bioaccumulation and assumes mercury and DDTR concentrations in invertebrates increase without an upper bound as soil concentrations increase. Results are presented in Section 4.0.

Cleanup goal recommendations are presented in Section 5.0.

2.0 ESTIMATION OF SEDIMENT PRGS

2.1 METHODOLOGY

Development of sediment PRGs associated with OU-2 was a multi-step process. The mercury and DDTR PRGs were developed using the BSAF method and the ratio method. The HCB PRG was developed by direct estimation of sediment concentration in the forward risk calculation to achieve an HI equivalent to 1. This direct calculation method for the HCB PRG is appropriate because HCB had an unacceptable risk associated only with incidental ingestion of sediment. The BSAF and ratio methods are used when risk to ecological receptors is primarily associated with the ingestion of fish.

The BSAF method paired fish tissue samples with associated sediment samples for mercury and DDTR within a defined home range for each fish type (i.e., forage fish and predatory fish). These data pairs were plotted and regression analyses were performed to determine an empirical relationship between the two media. The BSAF relationship between fish tissue and sediment concentrations is illustrative of the bioaccumulation of mercury from sediments through the various levels of the food chain and into fish tissue. This empirical relationship was ultimately used to predict a sediment concentration that would reduce tissue concentrations in site ecological receptors to acceptable risk levels.

The ratio method used a simplified approach to determine an empirical relationship between sediments and fish tissue. Fish tissue concentrations for the samples included in the RGO dataset (Section 2.3) were averaged to obtain a representative value in fish. Similarly, the sediment concentrations included in the RGO dataset were averaged to obtain a representative sediment value. The average fish tissue concentration (y) was divided by the average sediment value (x) to determine a ratio (R):

$$R = y / x \text{ or } y = Rx \quad \text{(Equation 1)}$$

The ratio describes the slope of a linear equation with a y-intercept of zero. This approach is a simplified description of bioaccumulation and assumes mercury and DDTR concentrations in fish increase without an upper bound as sediment concentrations increase.

The following sections provide additional information on the data that were selected for analysis, the process of pairing the site data, the regression analyses, and the estimation of sediment PRGs.

2.2 SELECTION OF AQUATIC ECOLOGICAL RECEPTORS FOR SEDIMENT PRG DEVELOPMENT

PRG development was designed to protect fish-eating birds that may forage in the Basin. USEPA proposed five receptors that were estimated to have current HIs greater than 1: mink, pied-billed grebe, great blue heron, little blue heron, and belted kingfisher. HIs were calculated for the five receptors using no observed adverse effect level (NOAEL) and lowest observed adverse effect level (LOAEL) toxicity reference values (TRVs) provided by USEPA (AMEC, 2011b).

USEPA proposed the mink as the receptor for the evaluation of risk to mammalian piscivores at OU-2. The results of the updated ERA (AMEC, 2011b) indicated that the mink had HIs greater than 1 from mercury and HCB. USEPA proposed the pied-billed grebe as the receptor for the evaluation of risk to insectivorous avian receptors at OU-2. The pied-billed grebe had HIs greater than 1 from methylmercury and DDTR. USEPA proposed three bird species for evaluating risk to avian piscivores at OU-2: the great blue heron, the little blue heron, and the belted kingfisher. These three receptors had HIs greater than 1 from methylmercury and DDTR. The great blue heron, little blue heron, and belted kingfisher represent the range of exposures to avian piscivores at OU-2. Great blue herons feed higher up the food chain and more opportunistically than little blue herons. Great blue herons also feed on larger fish that are not typically consumed by the little blue heron or the belted kingfisher. The little blue heron and belted kingfisher typically feed on smaller prey items. The great blue heron and little blue heron are suitable surrogate species to represent exposure to other avian piscivores at OU-2.

The belted kingfisher was selected as one of the representative species of piscivorous aquatic birds for quantification because this species is a year-round resident in Alabama. A range of exposure parameters from scientific literature is available for the belted kingfisher. The belted kingfisher was evaluated using two exposure scenarios in the ERA to account for the range of exposure parameters and site conditions at OU-2 (AMEC, 2011b). The first exposure scenario assumes that the belted kingfisher forages exclusively on forage fish obtained from the Basin and Round Pond. This assumption provides a highly conservative risk estimation that represents the maximum, or "worst-case," scenario. In the second exposure scenario, the dietary composition of the belted kingfisher is adjusted to reflect a more diverse diet that includes forage fish (51 percent), amphibians (25 percent), aquatic insects (19 percent), and crayfish (5 percent). This dietary makeup was obtained from the *Wildlife Exposure Factors Handbook* (USEPA, 1993) for belted kingfishers in a lake-type environment. The area use factor was also set to 0.5, representing a kingfisher that forages 50 percent of the time within OU-2 and 50 percent of the time outside OU-2. The

second exposure scenario represents a reasonable maximum exposure (RME) scenario for the belted kingfisher consistent with observed conditions at OU-2. Both scenarios were agreed to by USEPA, and are included in the RGO development for OU-2.

2.3 ANALYTICAL DATASET

The rationale for the data used in the PRG analysis for mercury, DDTR, and HCB is discussed in the following sections.

2.3.1 Mercury

Fish consumption by the pied-billed grebe, great blue heron, little blue heron, and belted kingfisher was determined to be one of the primary ecological risk drivers for mercury in the updated ERA (AMEC, 2011b). The dietary composition of the great blue heron includes both larger predatory fish and smaller forage fish. The pied-billed grebe, little blue heron, and belted kingfisher feed predominantly on forage fish. Therefore, the final dataset for the PRG estimation was separated into two datasets: one for predatory fish (represented by largemouth bass) and one for forage fish (represented by mosquitofish, bluegill, and brook silversides).

The dataset for mercury in predatory fish (Appendix A-1, Table A-1) includes the following:

- Whole-body largemouth bass samples collected from the Basin and Round Pond in 1994 and 2008
- Whole-body largemouth bass (weighted value based on 2001 filet and offal data) reported in the *OU2 RGO Support Sampling Report* (URS Corporation [URS], 2002)
- Whole-body largemouth bass samples collected in 1991 from BASF (formerly Ciba-Geigy) Whole-body largemouth bass samples collected in 1994 from the Stimpson Wildlife Refuge (Lake Hatchetigbee; reference area)
- Whole-body largemouth bass samples collected in 1994 from Tensaw Lake (reference area)
- Whole-body largemouth bass samples collected in 1994 from Three Rivers Lake (reference area)
- Basin sediment samples collected in 1991, 1994, 2001, and 2008
- Sediments collected in 1991 from BASF (formerly Ciba-Geigy)

- Sediment samples collected from the reference areas: Stimpson Wildlife Refuge (1994), Tensaw Lake (1994), and Three Rivers Lake (1994)

The dataset for mercury in forage fish (Appendix A-1, Table A-2) includes the following:

- Whole-body mosquitofish collected from the Basin and Round Pond in 1994 and 2001
- Whole-body bluegill collected from the Basin and Round Pond in 2008
- Whole-body silversides collected from the Basin and Round Pond in 2008
- Whole-body mosquitofish collected from the reference area in 1994
- Whole-body forage fish samples collected in 1994 from the Stimpson Wildlife Refuge (reference area)
- Whole-body forage fish samples collected in 1994 from Tensaw Lake (reference area)
- Whole-body forage fish collected in 1994 from Three Rivers Lake (reference area)
- Basin sediment samples collected in 1991, 1994, 2001, and 2008
- Sediment samples collected from the three reference areas: Stimpson Wildlife Refuge (1994), Tensaw Lake (1994), and Three Rivers Lake (1994)

2.3.2 DDTR

Consumption of aquatic insects and forage fish by the little blue heron, belted kingfisher, and pied-billed grebe is the primary ecological risk driver for DDTR. Aquatic insect and forage fish consumption was identified as the ecological risk driver for DDTR. The dietary composition of the little blue heron, belted kingfisher, and pied-billed grebe includes a substantial component of forage fish (represented by mosquitofish) and aquatic insects, as presented in the updated ERA (AMEC, 2011b). The final dataset for DDTR (Appendix A-1, Table A-3) includes the following:

- Whole-body mosquitofish collected from the Basin and Round Pond in 1994 and 2001
- Whole-body mosquitofish collected from the reference area (Lake Hatchetigbee) in 1994
- Whole-body forage fish samples collected in 1994 from the Stimpson Wildlife Refuge (reference area)
- Whole-body forage fish samples collected in 1994 from Tensaw Lake (reference area)

- Whole-body forage fish collected in 1994 from Three Rivers Lake (reference area)
- Individual and composite invertebrate samples collected from the OU-2 floodplain in 2010
- Basin sediment samples collected in 1991, 1994, and 2001
- Sediment samples collected from the three reference areas: Stimpson Wildlife Refuge (1994), Tensaw Lake (1994), and Three Rivers Lake (1994)

DDTR is a lipophilic compound. The reported fish tissue DDTR concentrations were lipid-normalized by dividing the reported DDTR concentrations by the fraction of lipids for each sample. Sediment DDTR concentrations were also normalized by dividing the reported DDTR concentrations by the average fraction of organic carbon (FOC) for the sediment samples.

2.3.3 HCB

HCB was identified as a COC in previous submittals of the ERA, with ecological risk stemming from ingestion of predatory fish. The predatory fish exposure point concentration (EPC) for HCB included in the updated ERA does not cause unacceptable risk to ecological receptors at OU-2 (AMEC, 2011b). Therefore, PRG analysis using the BSAF approach for this COC was unnecessary. HCB had unacceptable risk associated with incidental ingestion of sediments. A PRG for HCB was derived using an approach involving direct reduction in sediment concentration to achieve an HI of 1.

2.4 DATA PAIRING USED IN THE BSAF APPROACH

Paired observations in each dataset were made by matching fish samples either with collocated sediment samples or with sediment samples within a typical home range for each fish type. Data pairing of fish and sediment samples is the first step in BSAF development. Guidance in calculating the BSAF recommends that sediment samples across a typical foraging range be collected and analyzed, and that the sediment samples should be representative of the organism's immediate life history (Burkhard, 2009). Thus, appropriate tissue and sediment sample pairs are collected within a narrow timeframe (i.e., the same year). The use of sediment and tissue data across multiple years includes a time lapse between the exposed tissue and the medium in which the tissue was exposed. Fish may have also lived in various areas of the Basin during different life stages (i.e., juvenile vs. adult). Inclusion of data across multiple years increases the uncertainty associated with the data pairing. The data pairings used for the PRG development were generally for sediment and fish tissue samples collected within the same year. The

exception to this procedure includes pairing of sediments collected in 1991 and 1994 with fish tissue samples collected in 1991 and 1994. USEPA requested the 1991 data be included with the 1994 data. This deviation in the general data pairing methodology was made because the coefficient of determination (R^2) values obtained during linear regression analysis increased with inclusion of the older sediment data. The data pairings by Basin area and year are provided in Appendix A-2 and summarized below:

- Pairing 1991 and 1994 sediment with fish collected in 1991 and 1994
- Pairing 2001 sediments with fish collected in 2001
- Pairing 2008 sediments with fish collected in 2008

Analytical results for sediments within the foraging range of the organism were averaged in the data pairings to determine a representative concentration. Duplicate samples and multiple samples (up to six inches in depth) were averaged together in the data pairing process to obtain a representative concentration at a location. Sediment core samples in the 0 to 6 inch depth interval were treated as individual samples when averaging sediments at a location. Analytical results for fish tissue were averaged within a sample station if multiple samples were collected from a single location or area within the same year.

2.4.1 Sediment Concentrations Paired with Fish Concentrations

Sediment concentrations for mercury and DDTR were averaged based on fish home ranges. Predatory fish home ranges were assumed to encompass an entire quadrant of the Basin (i.e., northeast, northwest, southeast, and southwest) and the entire Round Pond. Surficial sediment samples collected within a single quadrant or area in a given year were averaged to calculate one representative concentration for that area. The individual fish samples for a given Basin quadrant or area and year were averaged to determine a representative tissue concentration for that Basin quadrant or area and year. Figure 2-0 shows the locations of the reference areas and Figures 2-1 to 2-3 shows the data pairings for predatory fish by year. One exception to this methodology was applied to the 1994 predatory fish sample results. The two 1994 predatory fish sample locations along the western shore of the Basin were centrally located near the dividing line between the northwest and southwest quadrant (Figure 2-1). The northernmost predatory fish sample location (OLE0103-0694) was paired in the northwest quadrant. The southernmost predatory fish sample location (OLE0102-0694), although in the northwest quadrant, was paired in the southwest quadrant. Sample OLE0102-0694 was collected near the division line between north and south, and the home range of fish collected at this location likely extends into the southwest quadrant. The average sediment concentration was paired with the average fish concentration for the same quadrant or area and

year in this approach. The sample was included in both quadrants, if the sample location was on the dividing line between two quadrants, due to the uncertainty associated with the sample's exact location. Figures 2-1 through 2-3 illustrate the Basin quadrant groupings of sediment and predatory fish samples by year. Individual analytical results are provided in Appendix A-1, Table A-1.

Forage fish home ranges were assumed to be a circle with a radius of 400 feet and centered on a sample station. This home range area is approximately 11.5 acres, which is greater than the average home range of a forage fish. This expanded home range was included for several reasons. The home range of a forage fish could be represented by various shapes arranged in multiple directions from the fish sample collection area. The 400-foot-radius circle was selected because it provided coverage in all directions and accounted for the uncertainty associated with the fish sample collection area in relation to the overall home range. All sediment data from Round Pond was paired with the forage fish data in Round Pond instead of using a 400-foot radius. This approach maximized the number of sediment samples associated with a given fish sample. Surficial sediment samples collected within the 400-foot radius, or along the boundary edge, were averaged to estimate a representative concentration for that area. Analytical results for fish tissue were averaged within a sample station if multiple samples were collected from a single location within the same year. Figures 2-4 through 2-6 illustrate the home ranges for forage fish and groupings of sediment and fish samples by year. Individual analytical results are provided in Appendix A-1, Tables A-2 and A-3. Sediments in each reference area were averaged to generate one representative concentration for the reference sediments. The average sediment concentration was paired with the average fish concentration for each reference area to generate one data point for each reference area. The reference areas were limited to one data pairing so that the OU-2 BSAF analysis would be representative of conditions in OU-2, rather than areas outside OU-2.

2.4.2 Methodology for Regression Analysis

The use of average fish tissue concentrations in regression analysis is more appropriate than use of individual fish tissue concentrations because multiple samples are present within an established forage area. Fish may swim over a larger range for which a single sediment sample at a capture location may not be fully representative. Averaging of fish tissue is advantageous because it reflects sediment/fish interactions across the range of that fish (not at the capture point only).

The number of subgroups and the resulting fit (R^2) were carefully considered. Two paired data points assure an R^2 of 1, but have little meaning. The pertinence of the regression equation increases as paired

data points are added. At least five paired data points are recommended for OU-2, including the reference areas. The five-point minimum for regression analysis is recommended based on several factors. Five points are considered to be:

- Enough points to visually check a scatter plot for evidence of a linear or non-linear relationship between the independent and dependent variables
- Enough points to visually check a scatter plot for evidence of outliers in x or y
- Sufficient data to test for suspected outliers (Dixon's test requires at least three points, but power to discriminate outliers increases quickly with additional points [ProUCL, V4.0].)
- Enough points to visually check a scatter plot for evidence of unequal variance in the dependent variable; e.g., increased scatter in y values as x values increase
- Enough points to visually check a normal probability plot for normality of the dependent variable (y)
- Sufficient data to test suspected non-normality of the dependent variable (Shapiro-Wilk's W-test can be run with as few points as n = 3, but additional points greatly increase the power [Gilbert, 1987])
- Enough points to visually check a normal probability plot for normality of residuals (the difference between the predicted value and the measured value of the dependent variable [y])
- Appropriate for visual inspection of a data plot. (For example, if there are three discordant points on the data plot, it is impossible to determine which one of the three is the outlier. With four points, it becomes possible to identify the discordant point if the other points are well-behaved. With five points on a chart, one discordant point is generally apparent upon inspection.)
- Sufficient data to test suspected non-normality of residuals
- Appropriate to increase the power of non-zero slope significance, which markedly increases with number of points greater than three

BSAFs were calculated to yield a Basin-wide PRG for DDTR and mercury. USEPA had suggested the potential of calculating BSAFs for different areas of OU-2. Available data for both chemicals were evaluated and determined to be limited if divided into subgroups by Basin area. Limitations inherent to the data pairings, when divided into subgroups, included the lack of availability of mercury data pairs for surficial sediment concentrations less than 20 mg/kg (the area of the graph that controls the PRG) and the small number of data pairs available in any given area (typically the number of data pairs was less than five for average fish by subgroup area for DDTR and mercury). When the dataset is subdivided by Basin

area, the resulting datasets are reduced in size, which would significantly reduce the power of results generated from the use of the smaller datasets.

2.5 PRG ANALYSIS

The mercury and DDTR data pairs were plotted in Microsoft® Excel format. Average sediment concentrations were plotted along the x axis, and the associated average fish concentrations were plotted along the y axis. A regression trend line, a R^2 value, and a p-value were calculated by Excel and placed on each graph. The goal was to find a model equation with an R^2 value greater than 0.7 and a p-value less than 0.05. Various forms of the regression relationship were evaluated because the exact form of the relationship between fish tissue and sediment concentrations was unknown. These forms include the linear and power regression models.

The ratio method was also used to calculate mercury and DDTR PRGs to provide a range of sediment PRGs for each receptor. The ratio method is not dependent on R^2 values or p-values, and has been used for PRG development when regression analysis does not indicate a strong correlation between the sediment and tissue data (as is indicated by R^2 values less than 0.7 and p-values greater than 0.05). R^2 values and p-values for the ratio method were not generated because the meaning of these two statistical terms for best fit lines is not equivalent to the meaning of these two terms for the ratio method. A discussion on these terms is provided in Appendix A-2 (Comparability of Statistical Parameters).

Tables 2-1 through 2-3b summarize the results of the power and linear regression analysis, including the resulting R^2 values, p-values, and regression equations, and the ratio method. Regression plots generated using the linear and power regression methods and ratio method are provided in Appendix A-1. Appendix A-3 presents the regression statistics, R^2 values, and p-values for each linear and power curve. The regression with the highest R^2 value (greater than 0.7) and acceptable p-value (less than 0.05) is identified for each relationship in the sections below.

2.5.1 PRG Analysis in Forage Fish

2.5.1.1 Mercury

The paired data, when plotted in Excel (Figure A-2a), showed an increasing trend at sediment concentrations below approximately 45 mg/kg, followed by a linear pattern with no significant slope at sediment concentrations greater than 45 mg/kg. This overall pattern shows bioaccumulation occurring at

sediment levels at or below 45 mg/kg with ecological systems reaching a state of equilibrium at mercury concentrations greater than 45 mg/kg. A segmented regression approach (i.e., separate regressions performed in two regions) was performed for the mercury data pairs for forage fish and predatory fish. The segmented regression approach may be applied when there is a defined shift in available data (Ryan, et al., 2007). A segmented regression plot is shown in Figure A-2b in Appendix A-2. Data pairs with sediment mercury concentrations greater than 45 mg/kg generate a relatively flat line with a slope not statistically different than zero, indicating an asymptotic condition or a plateau. Paired sediment data below 45 mg/kg for mercury were the focus of the regression analyses. Regression equations generated from this subset of data were used in the PRG development of mercury. Inclusion of the sediment data greater than 45 mg/kg would distort the regression equations for the area from 0-45 mg/kg and R^2 values would be less representative of bioaccumulation within the range of potential PRGs for OU-2. Multiple power and linear regression equations were generated for mercury in forage fish at sediment concentrations below 45 mg/kg using paired data for all species combined and by fish species. Each regression equation was analyzed with the inclusion of all three reference data points. Table 2-2a summarizes the R^2 values and p-values resulting from these scenarios, and Figures A-5a and A-5c in Appendix A-1 provide the regression plots for forage fish. Appendix A-3 presents the regression statistics, R^2 values, and p-values for each forage fish linear trend and power curve plotted in Figures A-5a and A-5c.

Table 2-2b summarizes the calculation of the tissue to sediment ratio for mercury, and Figure A-5b shows a graphical representation of the mercury ratio for OU-2. Only data pairs for sediment below 45 mg/kg of mercury were included in the ratio method for the reasons discussed above.

The R^2 values and p-values generated from the power and linear regression analyses achieved the USEPA goals of 0.7 and less than 0.05, respectively, and were considered in the PRG development for mercury. The ratio method was not carried forward in the PRG development for mercury because the power and linear models met the USEPA goals. The results of the power regression analyses indicate that bioaccumulation occurs to a larger degree in silversides and bluegills than in mosquitofish. The regression with the highest R^2 and acceptable p-value is the linear trend line for the mosquitofish (R^2 of 0.96 and p-value of 0.00008). Combining the species into one dataset provided a regression trend line between the three species. The combined dataset included 12 paired data points and yielded the R^2 value of 0.87 for the power regression with a p-value of 0.0000004, which met the USEPA goal of a R^2 value greater than 0.7, and acceptable p-values less than 0.05. The combined dataset is more representative of the foraging habits of the little blue heron and belted kingfisher, which select fish prey by size, not

species. The regression lines for the combined dataset are also representative of a more robust dataset, as demonstrated by the lower p-value, than the species-specific regression lines.

2.5.1.2 DDTR

Multiple regression models were also generated for DDTR in forage fish. DDTR data were available only for mosquitofish; therefore, separate species-specific curves were not generated like those for mercury. Separate regression analyses were conducted for DDTR in forage fish using normalized and non-normalized data. Normalization of the fish tissue data included dividing each fish tissue concentration by the associated sample's lipid fraction. The average normalized sediment concentration was calculated by dividing the average sediment concentrations by the average FOC of those sediment samples. Plots of the normalized and non-normalized data pairs are provided in Appendix A-1, Figures A-3a and A-3b. A distinct break in data trends was not observed at a threshold level as it was in mercury; therefore, all available DDTR data pairs were used in the regression analysis. Each regression line was generated with the inclusion of the three reference data points. Table 2-3a summarizes R^2 values and p-values resulting from the normalized and non-normalized scenarios, and Appendix A-1 (Figures A-6a and A-6c) provide the DDTR regression plots for forage fish. Table 2-3b summarizes the calculation of the tissue to sediment ratio for DDTR, and Figure A-6b shows a graphical representation of the DDTR ratio for OU-2. Appendix A-3 presents the regression statistics, R^2 values, and p-values for each forage fish linear trend and power curve plotted in Figures A-6a and A-6c.

Normalization of the data resulted in higher R^2 values and lower p-values than use of the non-normalized data. The power curve generated from the normalized data was the only DDTR regression equation that met the USEPA R^2 goal of 0.7 with a R^2 of 0.78 and an acceptable p-value of 0.0001. The power equation using normalized data was the only model included in the DDTR PRG development. The linear model and the non-normalized data model did not meet the USEPA R^2 goal of 0.7. The ratio method was not carried forward in the PRG development for DDTR because the power model met the USEPA goals. The use of a regression equation for normalized DDTR requires that fish data be normalized using the average lipid fraction for all samples, and the resulting sediment concentrations be de-normalized. De-normalization of sediments was accomplished by multiplying the normalized sediment concentration by the average FOC of all samples. The average fraction of lipids in fish (0.037) and the average FOC in sediments (0.055) were estimated from individual results presented in Appendix A-1 (Table A-3).

2.5.2 Regression Analysis in Predatory Fish

2.5.2.1 Mercury

The paired data, when plotted in Excel (Figure A-1a), showed a similar trend as forage fish (i.e., an increasing trend at sediment concentrations below approximately 45 mg/kg; a linear pattern with no significant slope at sediment concentrations greater than 45 mg/kg). This overall pattern shows bioaccumulation in predatory fish is also occurring at sediment levels at or below 45 mg/kg with ecological systems reaching a state of equilibrium or plateau at mercury concentrations greater than 45 mg/kg in sediment. A segmented regression approach was performed for the mercury data pairs for predatory fish. A segmented regression plot is shown in Figure A-1b in Appendix A-1. Data pairs with sediment mercury concentrations greater than 45 mg/kg generate a relatively flat line with a slope not statistically different than zero indicating an asymptotic condition or a plateau. Paired sediment data below 45 mg/kg for mercury were the focus of the regression analyses, and the regression equations generated from this subset of data were used in the PRG development of mercury. Multiple regression lines were generated for mercury in predatory fish by using paired data for all years combined and by sorting out data pairs by year (1991/1994, 2001, and 2008). Each scenario was analyzed with the inclusion of the five reference data pairs. Table 2-1 summarizes the R^2 values and p-values resulting from these scenarios, and Figures A-4a and A-4c in Appendix A-1, provides the regression plots for predatory fish. Figure A-4b shows a graphical representation of the mercury ratio for OU-2. Appendix A-3 presents the regression statistics, R^2 values, and p-values for each predatory fish linear trend and power curve plotted in Figures A-4a and A-4c.

The R^2 values and p-values for the power and linear regression analyses across all data groupings met the USEPA goals of a R^2 value greater than 0.7 and p-values less than 0.05. Therefore, each linear and power regression equation generated was included in the PRG development for mercury. The ratio method was not carried forward in the PRG development for mercury because the power and linear models met the USEPA goals. The linear regression analysis with the 2008 dataset provided the highest R^2 value (0.94) with an acceptable p-value of 0.00008. The R^2 value for the 1991/1994, 2001, and 2008 combined dataset using power regression analysis was 0.85 with acceptable p-value of 0.000002. The regression lines for the combined dataset are representative of a more robust dataset, as demonstrated by the lower p-value, than the year-specific regression lines.

2.6 PRG ESTIMATES – BSAF METHOD

Sediment PRGs were estimated once model equations were generated to correlate site sediment concentrations with fish tissue concentrations. The first step in this process was to determine an acceptable COC level that did not pose an unacceptable risk to aquatic ecological receptors at OU-2. Acceptable methylmercury and DDTR fish tissue concentrations were estimated by back calculating from risk equations presented in the updated ERA, in which the HI was set to 1. Back calculation of the NOAEL and LOAEL risk equations was performed to identify a range of target tissue concentrations. The geometric mean tissue concentration between the NOAEL and LOAEL range was selected as the target tissue concentration for PRG development.

The methylmercury concentration was assumed to conservatively reflect 100 percent of the total mercury in fish, and the target methylmercury concentration was assumed to also be the target total mercury concentration. The risk to ecological receptors from DDTR was attributed to fish and aquatic insects in the updated ERA (AMEC, 2011b). The aquatic insect dietary component for DDTR was assumed to be the 95 percent upper confidence limit (UCL) of the invertebrate data collected in 2010 and back calculation of risk equations was performed to identify target fish tissue concentrations. The 2010 invertebrate data includes emergent aquatic insects and were used as a representative concentration for aquatic insects in the back calculation of risk equations. The use of the 95 percent UCL for the invertebrate portion of diet for the selected aquatic receptors focuses the PRG development on the fish consumption pathway. Acceptable HCB concentrations in sediment were estimated by back calculating the NOAEL and LOAEL risk equations, in which the HI was set to 1, and determining the geometric mean sediment concentration between the two exposure scenarios. Summaries of the PRG concentrations that corresponded to a HI of 1 are presented for the five ecological receptors evaluated in Table 2-4. The NOAEL and LOAEL target predatory fish and target forage fish tissue concentrations, as shown on Table 2-4, are the same for methylmercury because the NOAEL and LOAEL toxicity reference values (TRVs) are the same. Equal NOAEL and LOAEL values result in the same geometric mean target fish tissue concentrations. The detailed back calculations for each constituent, including inputs and assumptions, are provided in Appendix B, Tables B-1 through B-8.

The aquatic receptors selected for PRG development were the belted kingfisher (assuming a highly conservative diet of 100% McIntosh Basin fish), belted kingfisher (reasonable maximum exposure [RME]), little blue heron, great blue heron, pied-billed grebe, and mink based on the results of the updated ERA (AMEC, 2011b). The minimum geometric mean target fish value (y) for these receptors

(Table 2-4) was entered into the equations listed on Tables 2-1, 2-2a, and 2-3a for mercury and DDTR, and then solved for a corresponding sediment concentration (x). Table 2-5 summarizes the NOAEL/LOAEL/geometric mean PRG results for mercury in predatory fish. The NOAEL and LOAEL TRVs for mercury are the same; equal values result in the same geometric mean. Table 2-6 summarizes the NOAEL/LOAEL/geometric mean PRG results for mercury in forage fish. Table 2-7 summarizes the NOAEL, LOAEL, and geometric mean PRG results for DDTR (normalized) for forage fish. Summaries of PRGs across the receptors are presented in Tables 2-8 to 2-10 for mercury risks from ingestion of predatory fish, mercury risk from ingestion of forage fish, and DDTR risk from ingestion of forage fish, respectively. The ratio method PRGs are presented on Tables 2-8 and 2-9 for informational purposes only to document the evaluation. The ratio method was not utilized in the development of the PRG range for mercury because the power and linear models met the USEPA goals for correlation coefficients and significance. The PRGs presented on Table 2-10 for DDTR are based on the power regression models of the normalized data. Figures 2-7 and 2-8 illustrate the range of PRGs for mercury and DDTR, respectively, across the different receptors.

The regressions with the highest R^2 values and significant p-values (< 0.05) were highlighted in yellow on Tables 2-5 through 2-10. Several regressions were highlighted in blue on the mercury tables (Tables 2-5, 2-6, 2-8, and 2-9). Blue highlighted regressions are considered adequate curve fits because of the availability of a more robust mercury dataset (demonstrated by a decrease in the p-value for these regressions). Mercury data were evaluated by species for forage fish and by year for predatory fish which reduced the robustness of the available data set and increasing the p-value for the regressions. Factors such as the species represented, number of data points, number of years of available data, and time of sampling should be considered along with the R^2 and p-values in selecting a relevant PRG based on a robust dataset. The use of all species data is representative of typical feeding habits of piscivorous receptors (i.e., piscivorous receptors do not select prey by species), and the use of data across all years captures changes over time.

2.6.1 Mercury

The range of mercury PRGs developed to be protective of ecological receptors ingesting forage and predatory fish is summarized below. This PRG range comprises the NOAEL-, LOAEL-, and geometric mean-based risks for mercury in sediment because these risk values are the same for mercury.

Mercury Sediment PRGs Protective of Ecological Receptors Ingesting Predatory Fish (Table 2-8):

- 1.0 mg/kg dw to 12 mg/kg dw for the great blue heron.

Mercury Sediment PRGs Protective of Ecological Receptors Ingesting Forage Fish (Table 2-9):

- 4.4 mg/kg dry weight (dw) to 20 mg/kg dw for the belted kingfisher (RME; assuming a diet consisting of fish and other dietary items and an area use factor of 50%);
- -0.043 mg/kg dw to 4.7 mg/kg dw for the belted kingfisher (assuming a highly conservative diet of 100% fish and an area use factor of 100%);
- 14 mg/kg dw to 109 mg/kg dw for the pied-billed grebe; and
- 1.2 mg/kg dw to 9.0 mg/kg dw for the little blue heron.

One negative PRG (-0.043) for linear regression of the bluegill dataset for the highly conservative belted kingfisher scenario is presented on Table 2-9 because the equation met the USEPA goals for the correlation coefficient (R^2 of 0.89) and p-value (0.001). Inclusion of this negative PRG value emphasizes the uncertainty in the use of the bluegill dataset alone with a linear regression model.

A separate mercury PRG for sediments was directly calculated based on risk to the mink. Risk for the mink was driven by direct ingestion of sediments and was not associated with the consumption of fish. Target risk-based mercury sediment concentrations were estimated by back calculating risk equations for the mink to a target sediment concentration associated with a HI of 1. The mercury sediment PRG for the mink is 27 mg/kg dw. Tables presenting this information are provided in Appendix B.

The ecological receptor with risk driven by the ingestion of predatory fish is the great blue heron. Mercury PRGs for the great blue heron ranged from 1.0 mg/kg dw to 12 mg/kg dw.

The most sensitive ecological receptors to mercury in forage fish are the belted kingfisher and the little blue heron. Mercury PRGs for the belted kingfisher ranged from -0.043 mg/kg dw to 20 mg/kg dw. Mercury PRGs for the little blue heron ranged from 1.2 mg/kg dw to 9 mg/kg dw.

2.6.2 DDTR

The range of DDTR PRGs developed to be protective of ecological receptors ingesting forage fish in OU-2 is summarized below. This PRG range comprises the NOAEL- to LOAEL-based risks for DDTR in sediment. The PRGs based on the geometric mean of the NOAEL- and LOAEL-based risks for DDTR in sediment are also discussed below.

DDTR Sediment PRGs Protective of Ecological Receptors Ingesting Forage Fish (Table 2-10):

- 0.69 mg/kg dw (NOAEL) to 1.2 mg/kg dw (LOAEL) for the belted kingfisher (RME; assuming a diet consisting of fish and other dietary items and an area use factor of 50%);
- 0.28 mg/kg dw (NOAEL) to 0.38 mg/kg dw (LOAEL) for the belted kingfisher (assuming a highly conservative diet of 100% fish and an area use factor of 100%);
- 0.37 mg/kg dw (NOAEL) to 1.2 mg/kg dw (LOAEL) for the pied-billed grebe;
- 0.48 mg/kg dw (NOAEL) to 0.71 mg/kg dw (LOAEL) for the little blue heron; and
- 1.3 mg/kg dw (NOAEL) to 2.1 mg/kg dw (LOAEL) for the great blue heron.

The belted kingfisher and the little blue heron are the most sensitive receptors to DDTR in sediments. The geometric mean DDTR PRGs are as follows:

- 0.91 mg/kg dw for the belted kingfisher (RME; assuming a diet consisting of fish and other dietary items and an area use factor of 50%):
- 0.33 mg/kg dw for the belted kingfisher (assuming a highly conservative diet of 100% fish and an area use factor of 100%);
- 0.58 mg/kg dw for the little blue heron;
- 0.66 mg/kg dw for the pied-billed grebe; and
- 1.7 mg/kg dw for the great blue heron.

DDTR is a unique COC at OU-2 because its source does not originate from within the Olin Property. Manufacturing activities at the Olin Plant did not include DDTR. The primary release mechanism for DDTR is migration of sediments and soils containing DDTR from the BASF property (formerly Ciba-Geigy), a Superfund site located immediately north of OU-2. Floodplain soil and sediment collected from the 1990s to 2010 at OU-2 show a distinct DDTR migration pattern. These data provide evidence that DDTR migrated as flood water receded south from the BASF property onto OU-2. Residual concentrations of DDTR in capped and uncapped soil/sediment on the BASF property range from 1 to 3 mg/kg, as reported by EPA during a conference call on December 6, 2011. Sediment samples collected from OU-2 in 2009 show that the DDTR concentrations at OU-2 are also within this same range (1 to 3 mg/kg). The BASF property has released DDTR to OU-2 in the past and may potentially release DDTR at these concentrations. It is not practical to maintain a PRG lower than 3 mg/kg at OU-2, as allowed by the Record of Decision for the BASF site, knowing that DDTR has and may continue to migrate to OU-2.

Upstream BASF DDTR concentrations of 1 to 3 mg/kg dw should be considered in risk management decisions in selection of the sediment DDTR clean up goal for OU-2 sediment.

2.6.3 HCB

A HCB PRG for sediments was developed by direct calculation of risk to the mink. Risk for the mink was driven by direct ingestion of sediments and was not associated with the consumption of fish. Target risk-based HCB sediments concentrations were estimated by back calculating risk equations for the mink to a target sediment concentration associated with a HI of 1. The HCB sediment PRG for mink is 7.6 mg/kg dw.

3.0 ESTIMATION OF TARGET SEDIMENT MERCURY CONCENTRATIONS USING SERAFM MODEL

3.1 INTRODUCTION

USEPA requested during a conference call on May 20, 2009 that the SERAFM model be used for OU-2. SERAFM is a process-based modeling system designed by USEPA to predict speciated mercury concentrations in water, sediments and fish tissue. SERAFM can be used to estimate HIs using these predictions and associated target sediment concentrations for a series of exposed wildlife species.

SERAFM is an alternate method to develop PRGs. Site-specific data, including mercury and methylmercury in surface water and sediment, were used to calibrate the SERAFM model. The model was used to predict a target sediment concentration below which the target receptors would not be exposed to sediment associated with HIs greater than 1. The five ecological receptors modeled in SERAFM are the same receptors evaluated using the direct calculation method or the BSAF method presented in Section 2.0 of this document. These receptors are the belted kingfisher, little blue heron, great blue heron, mink, and pied-billed grebe to match the receptors proposed by USEPA. Two dietary composition conditions were modeled for the belted kingfisher, as described in the ERA (AMEC, 2011b) and Section 2.2 of this document. The first dietary condition or highly conservative approach assumed 100% consumption of trophic level 3 fish (TL3) and a forage factor of 100%. The second dietary condition for reasonable maximum exposure assumed a modified diet that consisted of 35% trophic level 2 crayfish/frogs, 45% TL 3 fish, and 20% trophic level 4 fish and a forage factor of 50%. The inputs for both scenarios were agreed upon with USEPA. Suitable nesting habitat for and the number of belted kingfishers is limited at OU-2 as discussed in the ERA (AMEC, 2011b).

The following sections present the scenarios modeled, the methods used to select parameters for the model inputs, the calibration method, and model results. Model inputs and outputs are included in Appendix C.

3.2 SCENARIOS MODELED

Olin/AMEC and USEPA agreed to model two scenarios during a conference call on March 30, 2010. EPA further clarified the representations of these scenarios in conference calls conducted on December 6, 12, and 14, 2011.The two modeled scenarios are described below.

3.2.1 Scenario 1 – Six Feet NAVD88 Water Elevation

Scenario 1 assumed an OU-2 water elevation of 6 feet North American Vertical Datum 1988 (NAVD88). Six feet NAVD88 is the targeted minimum water elevation held since February 2009 at the OU-2 gate to reduce sediment resuspension. The analytical data used in this scenario consist of 2009 surface water, sediment (including fine sediment cores and sediment grab samples), porewater, and precipitation data. The Basin and Round Pond were modeled as one hydraulic unit, excluding the area of the deeper portion of the Basin. The center of the deeper portion of the Basin is defined as the area in the northwest portion of the Basin where the bathymetry shows a low elevation of approximately -36 feet NAVD88. The area of the deeper portion of the Basin, for the purposes of this model, is defined by transition of the epilimnion to the metalimnion at a water elevation of -13 feet NAVD88.

Inflow/outflow inputs were calculated using 2009 hydrology data and the area of the Basin and Round Pond, excluding the area of the deeper portions of the Basin. SERAFM uses a default hydraulic residence time (HRT) value, which along with volume, is used to estimate inflow and outflow (Appendix C). This HRT value was replaced in the model runs because inflow and outflow data were available. Scenario 1 represents a more typical flood year when a minimum water level is maintained.

Scenario 1 is presented with two sets of input values, where the inputs for 1) carbon associated with the phytoplankton concentration and 2) the Kd-bio: Kd-abio ratio were varied. All other input values were consistent within a given scenario. The input "phytoplankton concentration in Layer 1" in the first input set is the model default value of 1 gram per cubic meter (g/m^3), which represents eutrophic conditions and is the maximum value listed in the model documentation. The default value was used because the value (23.5 g/m^3), estimated from samples collected in the Basin, as reported in the 1996 Feasibility Study (WCC, 1996), does not produce reasonable model outputs and does not appear compatible with the model set up. The ratio of Kd-bio:Kd-abio is 17.8 in the first input set. This ratio is within the range of ratios produced by combining the lower and upper range values for Kd-bio and Kd-abio provided with the model documentation.

The "phytoplankton in Layer 1" input in the second set of input vales is 5 g/m^3. An input value greater than the default of 1 g/m^3 was recommended by the SERAFM author, Chris Knightes of USEPA, during a conference call on December 14, 2011. The Kd-bio:Kd-abio ratio is approximately 2.5 in the second input set.

3.2.2 Scenario 2 – Three Feet NAVD88 Water Elevation

Scenario 2 assumed an OU-2 water elevation of 3 feet NAVD88. A water elevation of 3 feet NAVD88 represents a low water level, as if the gate was not in use to maintain a minimum water level. The analytical data used in this scenario are 2008 surface water, sediment grab, and precipitation data. This scenario used 2009 porewater data because the 2009 porewater data set is the most contemporaneous data to 2008. The Basin and Round Pond were modeled as one hydraulic unit, excluding the area of the deeper portion of the Basin. Inflow/outflow inputs were calculated using 2008 hydrology data and the area of the Basin and Round Pond, excluding the area of the deeper portions of the Basin. Scenario 2 represents a drought year when a minimum water level is not maintained. Scenario 2 is presented with two sets of input values as discussed in Section 3.2.1.

3.3 PARAMETER SELECTION

A preliminary model was presented by Neptune and Company, Inc. (Neptune) during the December 7-8, 2009, meeting attended by Olin/AMEC and USEPA representatives. Neptune further refined their model inputs and presented the refinement with documentation of the changes on March 26, 2010. The Neptune inputs for SERAFM formed a basis for further evaluation of input parameters. Input parameters to SERAFM were further refined by Olin/AMEC for sensitive parameters. Inputs that were not sensitive were not changed. Selected parameters and justifications for input values are listed in Table 3-1.

3.4 MODEL CALIBRATION

The model was calibrated to match predicted outputs to measured values for OU-2 under Scenario 1 for both sets of inputs. The preliminary model provided by Neptune was calibrated so that actual measured site parameters matched mercury and methylmercury in sediment, which are not the most sensitive parameters for the final target sediment concentration predictions. Olin/AMEC calibrated the model provided by Neptune on October 15, 2010 to four parameters as recommended by the model developer in a conference call on December 14, 2011. The four parameters were filtered and unfiltered mercury and methylmercury concentrations in surface water. Calibration to measured filtered concentrations is considered more pertinent than calibration to unfiltered concentrations. The predicted outputs for the Olin/AMEC model for the four parameters were within an average of 31.2 percent (input set one) and 43.1 percent (input set two) of the measured values for OU-2 after calibration. A calibration target range of ± 50 to 100 % is considered acceptable to USEPA, based on the December 14, 2011 conference call.

The input parameters adjusted for calibration are noted in Table 3-1. The model-predicted output values for the four calibration targets are listed in Table 3-2 with the measured values and the relative percent differences between predicted and measured values.

3.5 SERAFM-PREDICTED TARGET SEDIMENT CONCENTRATIONS

The target sediment concentrations predicted by SERAFM for Scenario 1 are presented as ranges in Table 3-3. The ranges represent both sets of input values discussed in Sections 3.2.1 and 3.2.2. The target sediment mercury concentration ranges are 10.7 – 13.6 mg/kg dw for the little blue heron, 13.1 – 16.0 mg/kg dw for the great blue heron, 30.6 – 32.7 mg/kg dw for the mink, and 33.9 – 35.9 mg/kg dw for the pied-billed grebe. Target sediment concentration ranges for the belted kingfisher are 4.2 – 7.4 mg/kg dw and 14.8 – 17.6 mg/kg dw using the highly conservative diet/forage area and maximum reasonable diet/forage area, respectively. Suitable nesting habitat for and the number of belted kingfishers is limited at OU-2 as discussed in the ERA (AMEC, 2011b). The little blue heron, as a result, is recommended as a conservative representative ecological receptor for selection of a sediment PRG.

3.6 MODEL CONFIRMATION

A model is typically calibrated using a set of data, and the calibration is confirmed using an alternative set of data. The model is considered to be accurately predicting the system if the confirmation run predicts expected concentrations within an acceptable error range. It is not typical to use a confirmation run as a predictive tool; the confirmation run is used to evaluate the accuracy of the model using varying data sets.

The model developer recommended in a conference call on December 14, 2011 that once SERAFM was calibrated to Scenario 1, the model could be confirmed using the input parameters for Scenario 2. If the Scenario 2 values confirmed well with the calibrated Scenario 1 model, then the model would be confirmed. The model developer indicated that a reasonable calibration or confirmation error would be ±50% to 100%. Scenario 2 data were input into the calibrated Scenario 1 model. The average relative percent difference was 79.6% (input set one) and 75.1% (input set two), indicating that Scenario 2 confirmed the calibration of the model using Scenario 1. Predicting a target sediment concentration using Scenario 2 would not be a typical use of a confirmation run as described in the previous paragraph. However, predicted sediment target concentrations have been developed for Scenario 2 to provide an approximation of target concentrations under steady-state drought conditions resulting in a perpetual drought.

The Scenario 2 model indicated target sediment mercury concentration ranges of 2.0 to 12 mg/kg dw for the belted kingfisher based on the highly conservative diet/forage area and the maximum reasonable diet/forage area, respectively. Target sediment mercury concentration ranges were 6.7 – 9.2 mg/kg dw for the little blue heron, 8.5 – 10.9 mg/kg dw for the great blue heron, 15.4 – 16.5 mg/kg dw for the mink, and 17.1 – 18.2 mg/kg dw for the pied-billed grebe. These target sediment concentrations are not recommended as PRGs because the output for SERAFM under this scenario is representative of an infinite drought. This scenario is an extreme condition that is unlikely to occur. While a drought may last the duration of some receptor's lifespan, the system will have periods of non-drought conditions preceding and following the drought, which would allow the system to rebalance. Modeling an infinite, perpetual drought is an unnatural condition such that predictions from Scenario 2 are not recommended as mercury PRGs.

3.7 SENSITIVITY ANALYSIS

A sensitivity analysis was performed on the SERAFM model for Scenario 1 using the little blue heron as the ecological receptor and inputs that appeared sensitive. This analysis was performed by varying one input, while holding the remaining inputs constant. Inputs were varied by 80 and 120 percent (with the exceptions of lake area, particle size, and the mercury and methylmercury adsorption coefficients), and then predicted target sediment concentrations were compared. Lake area was varied by 90 and 110 percent because the areas of the Basin and Round Pond were based on the bathymetric and land surveys, which are expected to be within 10 percent of actual. Particle size was varied from 7 to 24 micrometers (µm) based on site-specific data. The mercury and methylmercury adsorption coefficients were varied by 10 and 1000 percent of the input value (1/10 and 10X of initial value) because these parameters are believed to vary more than the other parameters.

The input parameters selected and the results of the sensitivity analysis are listed in Tables 3-4a and 3-4b. Variability for Scenario 1, input set one ranged from -10.8 to +15.2% from the base target sediment concentration. Variability for Scenario 1, input set two ranged from -13.4% to +18.7% from the base target sediment concentration. The method of varying one parameter independently, while useful for exploring the sensitivity of the SERAFM model, is likely not representative of actual conditions at OU-2 as a whole. Changes to one parameter would likely result in simultaneous changes to other parameters. The variability reported in this sensitivity analysis should be used only to gauge the general representativeness of the model. The sensitivity analysis indicated that the results of the SERAFM model of OU-2 are representative of site conditions.

4.0 ESTIMATION OF A FLOODPLAIN SOIL PRG USING THE BSAF APPROACH

4.1 METHODOLOGY

The development of the PRGs for floodplain soils associated with OU-2 was a multi-step process. The soil PRGs for mercury and DDTR were developed using the methods outlined in Section 1.4. An HCB soil PRG was not estimated because the updated ERA results (AMEC, 2011b) indicated that HCB did not pose an unacceptable risk to terrestrial receptors.

The BAF approach is appropriate for mercury and DDTR because most terrestrial ecological risk stems from ingestion of invertebrates. The BAF relationship between insect tissue and soil concentrations is illustrative of the bioaccumulation of mercury from the soils into invertebrate tissue. The BAF method pairs insect tissue samples with associated floodplain soil samples for mercury and DDTR. The BAF approach is similar to the BSAF approach used in the sediment PRG evaluation. The data pairs have been plotted and regression analyses performed to assess whether an empirical relationship between the invertebrate tissue concentrations and soil concentrations is observed. This empirical relationship has been used to estimate a soil concentration that would reduce invertebrate concentrations and concentrations in receptors preying on invertebrates to acceptable risk levels. The ratio method was used, in addition to the BAF approach, to provide a range of acceptable soil PRGs for OU-2. The following sections outline the data that were selected for analysis, the process of pairing the site data, the regression analyses, and the estimation of soil PRGs.

4.2 SELECTION OF TERRESTRIAL ECOLOGICAL RECEPTORS FOR FLOODPLAIN SOIL PRG DEVELOPMENT

The development of soil PRGs has been designed to be protective of insectivorous birds that may forage in the OU-2 floodplains. The Carolina wren was selected as the receptor for the evaluation of risk to insectivorous birds at OU-2. The results of the updated ERA (AMEC, 2011b) indicate that the Carolina wren had an HI greater than 1 from methylmercury and DDTR. The Carolina wren has been selected as a conservative representative species of insectivorous terrestrial birds because its dietary intake is assumed to consist entirely (100 percent) of terrestrial invertebrates. Other terrestrial avian or mammalian receptors were not included in the development of the soil PRGs because unacceptable risks were not indicated, based on the updated ERA results (AMEC, 2011b).

4.3 ANALYTICAL DATASET

Invertebrate consumption by the Carolina wren has been determined to be one of the primary ecological risk drivers in the updated ERA (AMEC, 2011b). As stated above, the dietary composition of the Carolina wren is assumed to consist exclusively of invertebrates. The collection of floodplain soils, terrestrial insects, and spiders in July 2010 supported the Carolina wren food-web model. Historical terrestrial invertebrate data collected prior to 2010 are limited, and the available tissue and soil data were primarily either not collocated or not collected within the estimated home range for invertebrates. One insect out of nine collected in 1994 met the criteria for data pairing and was evaluated in the regression analyses for mercury and DDTR.

Per the updated ERA, risk is primarily associated with DDTR and methylmercury (AMEC, 2011b). Insect samples were not analyzed for methylmercury. A limited number of soil samples were analyzed for methylmercury during the July 2010 sampling effort, while all soil samples have been analyzed for mercury. Mercury data for insects and spiders were included in the BAF analysis for methylmercury using the USEPA-suggested ratio of 47 percent methylmercury and 53 percent inorganic mercury for total mercury in terrestrial insects.

4.4 DATA PAIRING

The typical home range of the Carolina wren is smaller than the area of OU-2; thus, data collected in the July 2010 sampling effort were included in the data set. Invertebrate samples were collected from six discrete locations throughout the OU-2 floodplain (Figure 4-1). Invertebrate samples were analyzed for mercury, methylmercury, and DDTR. Invertebrates collected at each sample location were divided into insect type (i.e., flying insect, crawling insect, and spiders) and composited to obtain a representative concentration for each insect type. Soil samples were also collected at each invertebrate sampling location and throughout the OU-2 floodplain as part of the collection effort. Data pairs were established by matching invertebrate samples with floodplain soil samples within 400 feet of the invertebrate collection site. A range of 400 feet was selected because a single soil sample at the capture location may not be fully representative of exposures to invertebrates. Invertebrates do not live exclusively in the place of capture and roam over a larger range. Duplicate soil samples were averaged together to get a representative soil concentration.

Two area-wide invertebrate samples were collected in addition to the six samples from discrete locations: one for the northeast Basin and one for the southeast Basin. The northeast area-wide sample included invertebrates collected from the three individual sampling locations in the northeast (OU2B-INS1-10, OU2B-INS2-10, and OU2B-INS3-10). The southeast area-wide sample included invertebrates collected from the two individual invertebrate sampling locations in the southeast (OU2B-INS5-10 and OU2B-INS4-10). Area-wide samples were also sorted and composited to obtain a representative concentration by insect type. Data pairs for the area-wide samples were established by matching the area-wide invertebrate results with the average soil result for the area. The data pairings for invertebrates and soils are provided in Appendix D, Tables D-1 and D-2. Figure 4-1 shows the data pairings for invertebrates and soils.

4.5 METHODOLOGY FOR REGRESSION ANALYSIS

The number of data pairs and the resulting fit (R^2) were carefully considered in the regression analysis for invertebrates and floodplain soil. Two paired data points ensure an R^2 of 1, but have little meaning. The pertinence of the regression equation increases as paired data points are added. At least five paired data points are recommended for OU-2. The five-point minimum for regression analysis is recommended based on several factors. Five points are considered to be:

- Sufficient points to visually check a scatter plot for evidence of a linear or non-linear relationship between the independent and dependent variables
- Sufficient points to visually check a scatter plot for evidence of outliers in x or y
- Sufficient data to test for suspected outliers (Dixon's test requires at least three points, but power to discriminate outliers increases quickly with additional points [ProUCL, V4.0].)
- Sufficient points to visually check a scatter plot for evidence of unequal variance in the dependent variable; e.g., increased scatter in y values as x values increase
- Sufficient points to visually check a normal probability plot for normality of the dependent variable (y)
- Sufficient data to test suspected non-normality of the dependent variable (Shapiro-Wilk's W-test can be run with as few points as n = 3, but additional points greatly increase the power [Gilbert, 1987].)
- Sufficient points to visually check a normal probability plot for normality of residuals (the difference between the predicted value and the measured value of the dependent variable [y])

- Appropriate for visual inspection of a data plot (For example, if there are three discordant points on the data plot, it is impossible to determine which one of the three is the outlier. With four points, it becomes possible to identify the discordant point if the other points are well-behaved. With five points on a chart, one discordant point is generally apparent upon inspection.)
- Sufficient data to test suspected non-normality of residuals
- Appropriate to increase the power of non-zero slope significance, which markedly increases with number of points greater than three

The data pairs were plotted in Microsoft® Excel format. Soil concentrations were plotted along the x axis, and the associated invertebrate concentrations were plotted along the y axis. A regression trend line and an R^2 value were calculated by Excel and placed on each graph. The goals were to find a model equation with an R^2 value greater than 0.7 and an acceptable p-value (i.e., a p-value less than 0.05). Various forms of the regression relationship were evaluated because the exact form of the relationship between invertebrate tissue and soil concentrations was unknown. These forms include both the linear and power regression models.

The ratio method was also used to calculate mercury and DDTR PRGs to provide a range of soil PRGs. The ratio method is not dependent on R^2 values or p-values, and is used for PRG development when regression analysis does not indicate a strong correlation between the soil and tissue data (indicated by R^2 values less than 0.7 and p-values greater than 0.05). R^2 values and p-values for the ratio method were not generated because the meaning of these two statistical terms for best fit lines are not equivalent to the meaning of these terms for the ratio method. A detailed discussion on the comparability of these terms is presented in Appendix A-2 (Comparability of Statistical Parameters).

Table 4-1a summarizes the results of the power and linear regression analyses, including the resulting R^2 values, p-values, and regression equations, and the ratio method. Regression plots generated using both the linear and power regression methods and plots of the ratio method are provided in Appendix D-1, Figures D-1a through D-5b. Appendix D-2 presents the regression statistics, R^2 values, and p-values for each linear and power analysis.

4.6 PRG ANALYSIS

4.6.1 Mercury

Multiple power and linear regression equations were generated for mercury in invertebrates. Regression equations for invertebrates were generated by using paired data for all tissue samples combined, and by invertebrate type (i.e., spiders, crawling insects, and flying insects). The historical data pair from 1994 was both included and excluded as part of the regression analysis of the combined dataset to measure the response of the R^2 values and p-values to this historical data pair. Table 4-1a summarizes the R^2 values and p-values resulting from these scenarios, and Appendix D-1, Figures D-1a, D-1c, D-2a, D-3a, D-4a, and D-5a, provide the regression plots for mercury in invertebrates. Appendix D-2 presents the regression statistics, R^2 values, and p-values for each linear and power analysis. Table 4-1b summarizes the calculation of the invertebrate tissue to soil ratio for mercury, and Figures D-1b, D-1d, D-2b, D-3b, D-4b, D-5b show a graphical representation of the mercury ratio for OU-2.

The results of the regression analysis indicate that bioaccumulation occurs to a larger degree in flying insects than in spiders and crawling insects. The observed R^2 values overall were well below the target of 0.7 set by USEPA and p-values were well above USEPA's target of 0.05. The highest R^2 value for the evaluated scenarios was for spiders (0.49) with a p-value of 0.5. The dataset for spiders is limited to three samples collected within a single sampling event (July 2010), which may account for the slightly higher R^2 values observed for spiders. The generally low R^2 values and high p-values generated from these regression analyses indicate that the regression models are poor indicators of future outcomes for mercury. Therefore, the ratio method, which does not depend on a R^2 value or p-value, was the method selected for development of the mercury soil PRG.

4.6.2 DDTR

Multiple power and linear regression equations were generated for DDTR in invertebrates. Regression equations for invertebrates were generated by using paired data for the combined tissue samples, by sorting samples by invertebrate type (i.e., crawling insects and flying insects). There were not enough data points to develop a regression equation for spiders only. Separate regression analyses for DDTR in invertebrates were generated using normalized and non-normalized data. Normalization of the data included dividing the invertebrate tissue concentrations by the sample lipid fraction, and dividing the floodplain soil concentrations by the sample FOC. Regression equations were also developed separately using the combined 1994 and 2010 insect and soil dataset. The analytical results for DDTR, fraction

lipids, and FOC are presented in Appendix D-1, Table D-2. Table 4-1a summarizes R^2 values and p-values resulting from the two scenarios, and Appendix D-1, Figures D-6a, D-6c, D-7a, D-7c, D-8a, D-8c, D-9a, D-9c, D-10a, and D-10c, provide the regression plots for DDTR in invertebrates. Appendix D-2 presents the regression statistics, R^2 values, and p-values for each linear and power analysis. Table 4-1c summarizes the calculation of the invertebrate tissue to soil ratio for DDTR, and Figures D-6b, D-6d, D-7b, D-7d, D-8b, D-8d, D-9b, D-9d, D-10b, and D-10d show a graphical representation of the DDTR ratio for OU-2.

Most regression equations did not achieve the USEPA R^2 goal of 0.7 and the USEPA p-value goal of less than 0.05. The only exception was the scenario using non-normalized flying insect tissue and non-normalized soil data which achieved an R^2 value of 0.92 (power) with an acceptable p-value of 0.04. The typical dietary intake of a Carolina wren includes a more varied diet than just flying insects so using this invertebrate class alone would not yield a suitable PRG. The Carolina wren is a ground forager and would likely consume a much higher proportion of crawling insects and spiders than flying insects. This adds to the level of uncertainty associated with PRGs based on ingestion of flying insects only. Flying insects also may include emergent aquatic insects, and remedial activities for OU-2 sediments will likely serve to reduce insect mercury concentrations because a significant portion of insects spend their larval stages in a sediment environment. Normalized data are also more appropriate for lipophilic compounds, such as DDTR. For these reasons, the ratio method, using normalized data, was selected as most appropriate for the development of the DDTR soil PRG.

4.7 RANGE OF FLOODPLAIN SOIL PRG ESTIMATES

4.7.1 Mercury

Floodplain soil PRGs for mercury were estimated using the ratio method to correlate site soil concentrations with invertebrate tissue concentrations. Floodplain soil PRGs using the linear and power regression equations were also estimated for informational purposes only to document the evaluation because the power and linear analyses did not achieve the USEPA goals for R^2 values greater than 0.70 and p-values (i.e., p-values less than 0.05). The first step in this process was to determine an acceptable COC level that did not pose an unacceptable risk to the Carolina wren. An acceptable methylmercury and DDTR invertebrate tissue concentration was estimated by back-calculating from risk equations presented in the updated ERA, in which the HI was set to 1. A summary of the PRG concentrations that corresponded to an HI of 1 is presented for the Carolina wren in Table 4-2. The NOAEL and LOAEL

target invertebrate concentrations for mercury are the same because the NOAEL and LOAEL TRVs are the same, resulting in equal NOAEL, LOAEL, and geometric mean target concentrations, as shown on Table 4-2.

The back-calculations of methylmercury risk equations are provided in Appendix E, Tables E-1 to E-2. A target mercury concentration in invertebrate tissues was determined by assuming that 47 percent of total mercury is in the form of methylmercury in invertebrates. Dividing the target methylmercury concentration by 47 percent provided an associated total mercury concentration in invertebrate tissue. The selected target methylmercury concentration in invertebrate tissue was 0.076 mg/kg, and the selected target total mercury concentration was 0.16 mg/kg (Table 4-2).

Ratio method soil PRGs were calculated by entering the target methylmercury value (y) for invertebrates (0.076 mg/kg) into Equation 1 (Section 2.1) and solving for a corresponding soil mercury concentration (x). The resulting soil mercury NOAEL/LOAEL/geometric mean- based PRGs protective of the Carolina wren ranged from 0.54 mg/kg dw to 1.9 mg/kg dw using the ratio method (Table 4-3). Floodplain mercury soil concentrations in this range are likely to yield an acceptable level of methylmercury in the terrestrial food web. A summary of the mercury PRGs developed for floodplain soils is provided in Table 4-5. The ratio method equations were highlighted in green on Tables 4-3 and 4-5 to indicate the equation is considered appropriate for PRG development because regression analyses did not achieve the USEPA goals for statistical relevance. Figure 4-2 illustrates the range of mercury PRGs calculated by the ratio method for each invertebrate grouping.

4.7.2 DDTR

Floodplain soil PRGs for DDTR were estimated using the ratio method to correlate site soil concentrations with invertebrate tissue concentrations, as well as linear and power regression equations, using normalized and non-normalized data. The non-normalized flying insect data grouping was the only model that met the USEPA R^2 goal of 0.7 and the USEPA p-value goal of less than 0.05. There is uncertainty in the linear and power regression equations based on the ingestion of flying insects only and the use of non-normalized data for lipophilic compounds such as DDTR; thus, PRGs using non-normalized data and the linear and power regression models were presented for informational purposes only to document the evaluation.

DDTR is a lipophilic chemical. To calculate the PRG of a lipophilic chemical like DDTR the data are normalized by dividing tissue concentrations by the lipids fraction and soil concentrations by FOC. The target DDTR value for invertebrates was normalized by dividing the target DDTR tissue concentration by the average lipid fraction from the July 2010 insect samples prior to insertion into Equation 1 for the ratio method. Equation 1 was then solved for a corresponding normalized soil concentration (x). The normalized soil concentration (x) was then denormalized by multiplying by the average FOC in July 2010 floodplain soil samples. Comprehensive data groupings were evaluated (i.e., individual invertebrate types or groups of invertebrates) to provide a range of potential soil DDTR PRGs. The back-calculations of DDTR risk equations are provided in Appendix E, Table E-3. Ratio method soil PRGs were calculated by entering the target DDTR value (y) for invertebrates (0.18 mg/kg) into Equation 1 (Section 2.1) and solving for corresponding soil NOAEL-, LOAEL-, and geometric mean-based DDTR concentrations (x) (Tables 4-4a, 4-4b, and 4-4c, respectively). A summary of the NOAEL-, LOAEL-, and geometric mean-based DDTR PRGs developed for floodplain soils is provided in Table 4-6. The ratio method equations were highlighted in green on these tables to indicate that the equation is considered appropriate for PRG development because the power and linear analyses did not achieve USEPA statistical goals for relevance.

Figure 4-3 illustrates the range of DDTR PRGs calculated by the ratio method for each invertebrate grouping. The resulting normalized NOAEL to LOAEL soil DDTR PRGs protective of the Carolina wren ranged from 0.032 mg/kg dw to 0.31 mg/kg dw. The resulting geometric mean soil DDTR PRGs protective of the Carolina wren ranged from 0.039 mg/kg dw to 0.25 mg/kg dw. Floodplain DDTR soil concentrations in this range are likely to yield an acceptable level of DDTR in the terrestrial food web.

Remedial activities for OU-2 sediments are likely to reduce insect DDTR concentrations because a significant portion of insects spend their larval stages in a sediment environment. DDTR is a unique COC at OU-2 because its source does not originate from within the Olin Property. Manufacturing activities at the Olin Plant did not include DDTR. The primary release mechanism for DDTR is migration of sediments and soils containing DDTR from the BASF property (formerly Ciba-Geigy), a Superfund site located immediately north of OU-2. Floodplain soil and sediment collected from the 1990s to 2010 at OU-2 show a distinct DDTR migration pattern. These data provide evidence that DDTR migrated as flood water receded south from the BASF property onto OU-2. Residual concentrations of DDTR in capped and uncapped soil/sediment on the BASF property range from 1 to 3 mg/kg, as reported by EPA. Floodplain soil samples collected from OU-2 in 2010 show that the DDTR concentrations at OU-2 are also within this same range (1 to 3 mg/kg). The BASF property has released DDTR to OU-2 in the past

and may potentially release DDTR at these concentrations. It is not practical to maintain a PRG lower than 3 mg/kg at OU-2, as allowed the Record of Decision for the BASF site, knowing that DDTR has and may continue to migrate to OU-2. Upstream BASF DDTR concentrations of 1 to 3 mg/kg dw should be considered in risk management decisions in selection of the DDTR cleanup goal for OU-2 soil.

5.0 SUMMARY AND RECOMMENDATIONS

The purpose of this RGO document is to present PRGs that have been developed for mercury, HCB, and DDTR in sediment and floodplain soils. PRGs for sediment were calculated using four methods: BSAF approach, the ratio method, direct calculation of the PRG from risk equations, and SERAFM. PRGs for floodplain soils were calculated using the ratio method.

The process for estimating sediment and floodplain soil PRGs began with the forward risk calculations based on COC data and conservative underlying assumptions. Several layers of assumptions are used in forward risk calculations, and, for each layer, a conservative value is used to represent exposure. The resulting sediment and soil PRGs that were estimated by back calculating to acceptable risk levels are conservative because the exposure assumptions are multiplicative.

Sediment PRGs Based On BSAF Approach

Mercury and DDTR sediment (in dry weight) PRGs were estimated using the BSAF method as one approach. The BSAF approach paired average sediment concentrations with average fish tissue concentrations within an estimated home range for each fish type. Regression analyses that met USEPA's goals for correlation coefficients (i.e., R^2 greater than 0.7) and significance (i.e., p-value less than 0.05) were acceptable. Separate analyses were conducted for predatory fish and forage fish. Both power and linear regression equations were generated for each fish type.

Ratios for mercury and DDTR bioaccumulation, based on the average tissue concentrations and average sediment concentrations, were calculated as a second approach. The ratio method was utilized in the development of a PRG range for mercury or DDTR because the power and linear models met the USEPA goals for correlation coefficients and significance. Ratio method PRGs for mercury are presented for informational purposes only to document the evaluation. The results from the BSAF approach give a range of sediment PRGs for each receptor.

Mercury Sediment PRGs

The R^2 values associated with the power and linear regression equations for mercury were greater than 0.7 and demonstrated acceptable p-values (i.e., less than 0.05) for both predatory fish and forage fish. Target risk-based fish tissue concentrations were estimated by back calculating risk equations to a target

fish tissue concentration associated with a HI of 1 for four sensitive piscivorous receptors (belted kingfisher, little blue heron, great blue heron, and pied-billed grebe). The belted kingfisher was evaluated using two scenarios to capture the range of dietary and area use factors available in scientific literature. One scenario assumed a belted kingfisher lived and foraged exclusively on fish within the Basin/Round Pond, representing a highly conservative approach. The second scenario assumed a reasonable maximum exposure approach using a varied diet (including amphibians and crayfish) and a portion of time (50%) spent foraging outside of the Basin. The inputs for both scenarios were agreed upon with USEPA. Suitable nesting habitat for and the number of belted kingfishers is limited at OU-2 as discussed in the ERA (AMEC, 2011b). A mercury PRG for sediment was also calculated using the ratio method for each receptor for informational purposes only to document the evaluation. The target fish tissue concentration for mercury was divided by the bioaccumulation ratio to determine the associated target sediment concentration for mercury. The range of mercury PRGs developed to be protective of ecological receptors ingesting fish using the BSAF approach is summarized below. This PRG range comprises the NOAEL-, LOAEL-, and geometric mean-based risks for mercury in sediment because the NOAEL and LOAEL TRVs are the same for mercury.

Mercury Sediment PRGs Protective of Ecological Receptors Ingesting Predatory Fish:

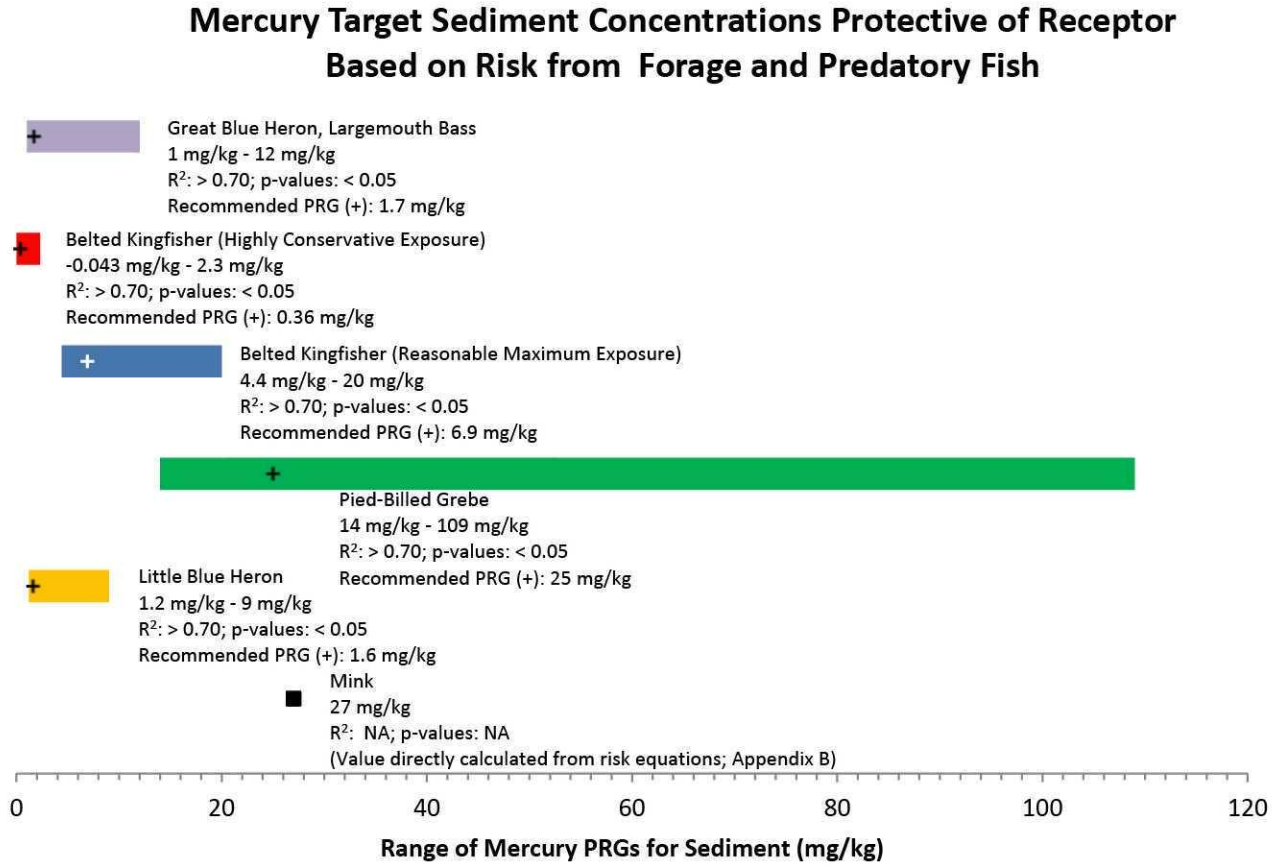
- 1.0 mg/kg dw to 12 mg/kg dw for the great blue heron.

<u>Mercury Sediment PRGs Protective of Ecological Receptors Ingesting Forage Fish:</u>

- 4.4 mg/kg dw to 20 mg/kg dw for the belted kingfisher (assuming a diet consisting of fish and other dietary items and an area use factor of 50%);
- -0.043 mg/kg dw to 4.7 mg/kg dw for the belted kingfisher (assuming a diet of 100% fish and an area use factor of 100%);
- 14 mg/kg dw to 109 mg/kg dw for the pied-billed grebe; and
- 1.2 mg/kg dw to 9.0 mg/kg dw for the little blue heron.

A separate mercury PRG for sediments was directly calculated based on risk to the mink. Risk for the mink was driven by direct ingestion of sediments and was not associated with the consumption of fish. Target risk-based mercury sediments concentrations were estimated by back calculating risk equations for the mink to a target sediment concentration associated with an HI of 1. The mercury sediment PRG for the mink is 27 mg/kg dw.

The most sensitive ecological receptors to mercury in forage fish are the belted kingfisher and the little blue heron. The figure below shows the range of mercury PRGs by ecological receptor. Mercury PRGs for the belted kingfisher ranged from -0.043 mg/kg dw to 20 mg/kg dw. The negative PRG value is illustrative of the conservative nature of developing a PRG using only one forage fish species and assuming that the belted kingfisher forages exclusively in the Basin on that one species. Mercury PRGs for the little blue heron ranged from 1.2 mg/kg dw to 9 mg/kg dw. Mercury PRGs ranged from 14 mg/kg dw to 109 mg/kg dw for the pied-billed grebe. The ecological receptor with risk driven by the ingestion of predatory fish is the great blue heron. Mercury PRGs for the great blue heron ranged from 1.0 mg/kg dw to 12 mg/kg dw.



+ Indicates the PRG for the receptor using the combined dataset (Table 2-8 and Table 2-9).

DDTR Sediment PRGs

Concentrations obtained from the power regression analysis of normalized data were included in the range of sediment DDTR PRGs. The range of DDTR PRGs protective of ecological receptors ingesting forage fish in OU-2 is summarized below. This range comprises the PRGs based on NOAEL- to LOAEL-based risks for DDTR in sediment. The PRGs based on the geometric mean of the NOAEL- and LOAEL-based risks for DDTR in sediment are also discussed below.

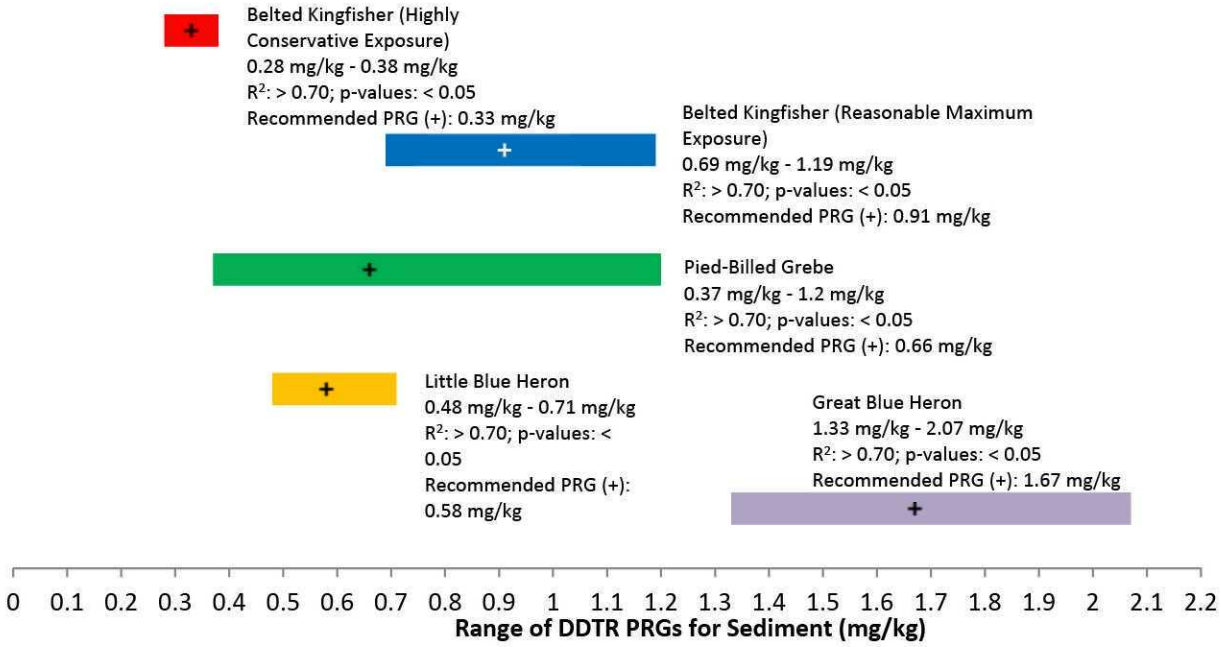
DDTR Sediment PRGs Protective of Ecological Receptors Ingesting Forage Fish (Table 2-10):

- 0.69 mg/kg dw (NOAEL) to 1.2 mg/kg dw (LOAEL) for the belted kingfisher (RME; assuming a diet consisting of fish and other dietary items and an area use factor of 50%)
- 0.28 mg/kg dw (NOAEL) to 0.38 mg/kg dw (LOAEL) for the belted kingfisher (assuming a highly conservative diet of 100% fish and an area use factor of 100%);
- 0.37 mg/kg dw (NOAEL) to 1.2 mg/kg dw (LOAEL) for the pied-billed grebe;
- 0.48 mg/kg dw (NOAEL) to 0.71 mg/kg dw (LOAEL) for the little blue heron; and
- 1.3 mg/kg dw (NOAEL) to 2.1 mg/kg dw (LOAEL) for the great blue heron.

The belted kingfisher and the little blue heron are the most sensitive receptors to DDTR in sediments. The geometric mean DDTR PRGs are as follows:

- 0.91 mg/kg dw for the belted kingfisher (RME; assuming a diet consisting of fish and other dietary items and an area use factor of 50%):
- 0.33 mg/kg dw for the belted kingfisher (assuming a highly conservative diet of 100% fish and an area use factor of 100%);
- 0.58 mg/kg dw for the little blue heron;
- 0.66 mg/kg dw for the pied-billed grebe; and
- 1.7 mg/kg dw for the great blue heron.

DDTR Target Sediment Concentrations Protective of Receptor Based on Risk from Forage Fish



+ Indicates the geometric mean PRG for the receptor (Table 2-10).

The primary release mechanism for DDTR is migration of sediments and soils containing DDTR from the BASF property (formerly Ciba-Geigy). Post-remediation, upstream BASF DDTR concentrations of 1 to 3 mg/kg dw should be considered in risk management decisions in selection of the sediment DDTR clean up goal for OU-2 sediment.

HCB Sediment PRG

A HCB PRG for sediments was developed by direct calculation of risk to the mink. Risk for the mink was driven by direct ingestion of sediments and was not associated with the consumption of fish. Target risk-based HCB sediments concentrations were estimated by back calculating risk equations for the mink to a target sediment concentration associated with an HI of 1. The recommended HCB sediment PRG for mink is 7.6 mg/kg.

Sediment PRGs Based on SERAFM Modeling

Mercury PRGs were also estimated using the SERAFM model developed by USEPA. SERAFM was populated with site-specific inputs from surficial sediments and surface water in the Basin and Round Pond. Two scenarios were modeled for sediment in the Basin and Round Pond. Scenario 1 represents a typical flood year using a minimum 6-foot water elevation and 2009 data. Scenario 2 represents a drought using a minimum 3-foot water elevation and 2008 data. Scenario 1 was used to calibrate SERAFM, and Scenario 2 was used as confirmation of the model calibration. The model confirmed well for Scenario 2. The two receptors with the lowest PRGs using SERAFM were the belted kingfisher and little blue heron. The PRGs developed for the belted kingfisher ranged from 4.2 to 7.4 mg/kg dw for the highly conservative exposure scenario and 14.8 to 17.6 mg/kg dw for the reasonable maximum exposure scenario. SERAFM predicted a range of sediment PRGs from 10.7 to 13.6 mg/kg dw for the little blue heron. Suitable nesting habitat for and the number of belted kingfishers is limited at OU-2 as discussed in the ERA (AMEC, 2011b).

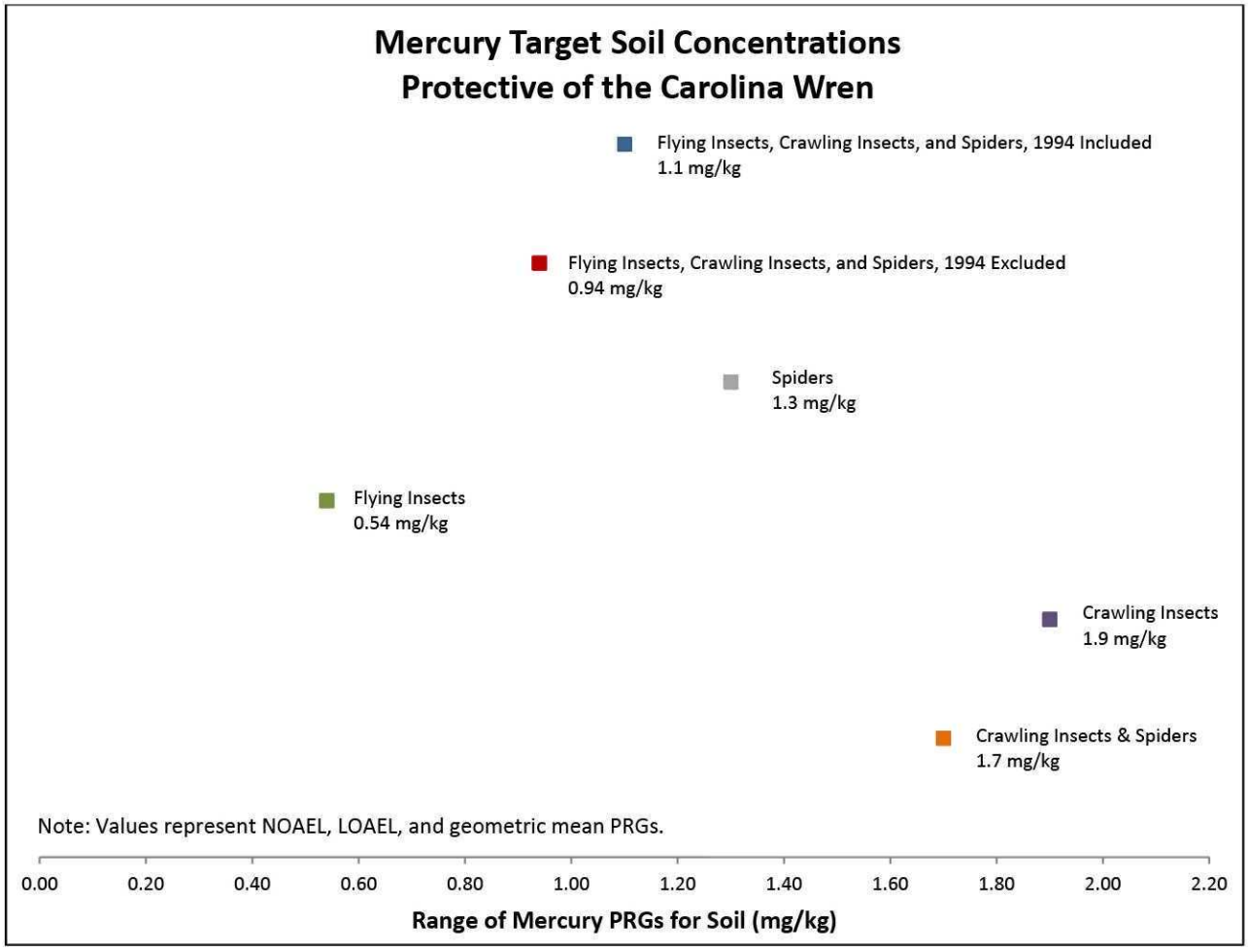
The cleanup goal for mercury in sediment predicted by SERAFM ranges from 4.2 mg/kg dw to 17.6 mg/kg dw. This range encompasses the SERAFM cleanup goals predicted for the little blue heron (10.7 to 13.6 mg/kg dw).

Mercury Floodplain Soil PRGs Based on the Ratio Method

Mercury floodplain soil PRGs were estimated using the ratio method. Floodplain soil PRGs for mercury using the linear and power regression equations were also estimated for informational purposes only to document the evaluation because the power and linear analyses did not achieve the USEPA goals for statistical relevance. Invertebrate data were separated into multiple groupings to provide a range of soil mercury PRGs. Data groupings included tissue and soil data pairs from individual invertebrate types (i.e., flying insects, crawling insects, and spiders) and from groups of these invertebrates (i.e., all invertebrate types combined as well as the combination of crawling insects and spiders only).

The PRGs were estimated by back-calculating to a target invertebrate tissue methylmercury concentration associated with a HI of 1 for insectivorous avian receptors identified for OU-2 (i.e., the Carolina wren). Methylmercury in insect tissue was the primary risk driver to the Carolina wren in the updated ERA. The target invertebrate tissue methylmercury concentration was divided by a bioaccumulation ratio determined from the average methylmercury tissue and average soil mercury concentration to obtain a

range of NOAEL-, LOAEL-, and geometric mean-based soil PRGs for mercury. The NOAEL and LOAEL target invertebrate concentrations are the same for mercury because the NOAEL and LOAEL TRVs are the same, resulting in the same value for the geometric mean. NOAEL/LOAEL/geometric mean soil mercury PRGs protective of the Carolina wren ranged from 0.54 mg/kg to 1.9 mg/kg using the ratio method.



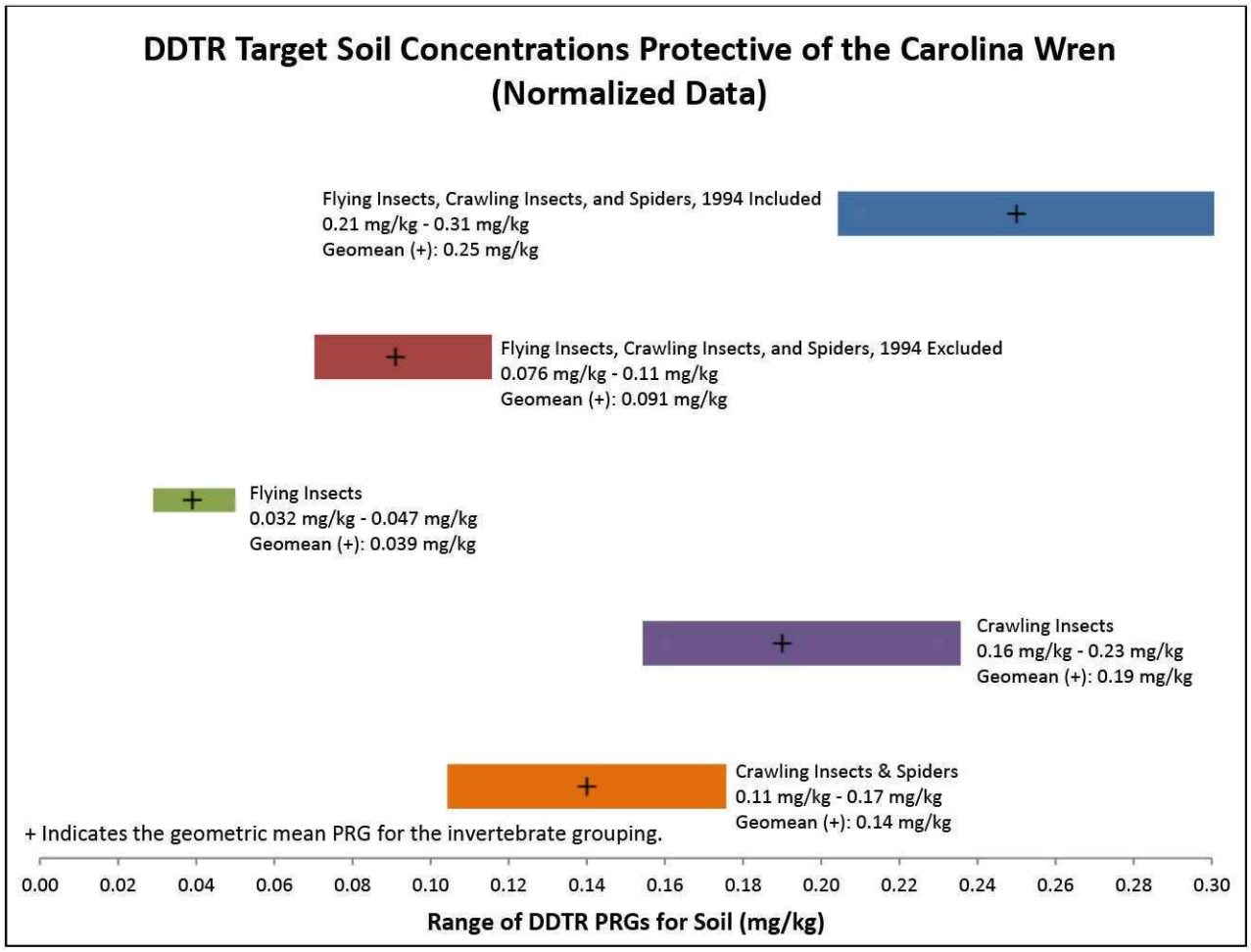
The mercury PRGs for floodplain soils were developed using highly conservative exposure assumptions. The flying insects provide a mercury PRG of 0.54 mg/kg. This invertebrate class does not represent the typical dietary intake of a Carolina wren. The Carolina wren is a ground forager and would likely consume at least some proportion of crawling insects and spiders. This adds to the level of uncertainty in considering PRGs developed based on flying insects alone. Flying insects also include emergent aquatic insects, and remedial activities for OU-2 sediments will likely serve to reduce insect mercury

concentrations because a significant portion of insects spend their larval stages in a sediment environment.

DDTR Floodplain Soil PRGs Based on the Ratio Method

DDTR floodplain soil PRGs were evaluated using the ratio method, similar to the development of soil mercury PRGs, but with normalized and non-normalized data. Floodplain soil PRGs for DDTR were also estimated using the linear and power regression equations using normalized and non-normalized data for informational purposes only to document the evaluation. The non-normalized flying insect data grouping was the only model that met the USEPA R^2 goal of 0.7 and the USEPA p-value goal of less than 0.05. There is uncertainty in the linear and power regression equations based on the ingestion of flying insects only and the use of non-normalized data for lipophilic compounds such as DDTR. PRGs using non-normalized data and the linear and power regression models were estimated for informational purposes only to document the evaluation. All data groupings were evaluated (i.e., individual invertebrate types or groups of invertebrates) to provide a range of potential soil DDTR PRGs.

The PRGs were estimated by back-calculating to a target DDTR invertebrate tissue concentration associated with a HI of 1 for insectivorous avian receptors (i.e., the Carolina wren). The target invertebrate tissue DDTR concentration was divided by a bioaccumulation ratio determined from the average DDTR tissue and average soil DDTR concentration to obtain a range of NOAEL-, LOAEL-, and geometric mean-based soil PRGs for DDTR. The NOAEL-, LOAEL-, and geometric mean-based soil DDTR PRGs protective of the Carolina wren ranged from 0.032 mg/kg to 0.31 mg/kg using the ratio method with normalized data. The geometric mean soil DDTR PRG range protective of the Carolina wren ranged from 0.039 mg/kg to 0.25 mg/kg using the ratio method.



A DDTR PRG for floodplain soils was developed using highly conservative exposure assumptions. The DDTR LOAEL HI for the Carolina wren was 1.4 in the updated ERA, which is slightly above the target value of 1. The conservative nature of the risk equations would indicate that the DDTR HI of 1.4 is likely overestimated for the Carolina wren. This adds to the level of uncertainty for the need for a DDTR PRG for floodplain soils. Remedial activities for OU-2 sediments will likely reduce insect DDTR concentrations because a significant portion of insects spend their larval stages in a sediment environment. Manufacturing activities at the Olin Plant did not include DDTR. The primary release mechanism for DDTR is migration of sediments and soils containing DDTR from the BASF property. Post remediation, upstream BASF DDTR concentrations of 1 to 3 mg/kg dw should be considered in risk management decisions in selection of the sediment DDTR clean up goal for OU-2 sediment.

RECOMMENDATIONS

Selection of PRGs is a risk management decision that is based on a number of considerations. The following facts should be considered. The Basin and Round Pond constitute unique water bodies, unlike other systems for which PRGs have been generated in the past. The Basin and Round Pond:

- Are on private property associated with an active operating facility owned by Olin;
- Are hydraulically controlled by an engineered structure (the berm and gate system) that maintains water levels to reduce resuspension;
- Are restricted from human exposure because of Olin's continuous surveillance and physical barriers to restrict trespassers;
- Are limited for fish passage to the river by the berm and gate system; and
- Exhibit a relatively low percentage of methylmercury in relation to total mercury compared to comparable environments, as described in the RI Addendum (AMEC, 2011a).

Overflow from the Basin and Round Pond does not cause an exceedance of the ambient water quality criterion (AWQC) of 0.012 microgram per liter (µg/L) in the river under the conditions sampled. This statement is based on a mass balance calculation that included mercury concentrations and flow rate from the overflow and river (AMEC, 2011a).

Recommended Sediment PRGs

The following PRGs are recommended as remedial goals.

The mercury PRG for sediment using the BSAF approach is 1.6 mg/kg dw based on risk to the little blue heron. The mercury PRG of 1.6 mg/kg was calculated using the power regression equation and includes data from all forage fish species. The PRG for mercury in sediment predicted by SERAFM is approximately 10.7 – 13.6 mg/kg dw based on the little blue heron. The SERAFM PRG value of 10.7 mg/kg mercury is realistic as a cleanup goal due to the conservative nature of the underlying risk parameters (i.e., toxicity values, exposure frequency, etc.). It is recommended that a cleanup goal range of 1.6 to 10.7 mg/kg be applied to OU-2 sediment.

The recommended sediment cleanup goal for DDTR is 3 mg/kg based on upgradient concentrations that that are acceptable to EPA, as discussed above. The recommended cleanup goal for HCB is 7.6 mg/kg based on risk to the mink. The recommended cleanup goals for sediment are listed below.

- Mercury: 1.6 to 10.7 mg/kg
- DDTR: 1 to 3 mg/kg
- HCB: 7.6 mg/kg

The distribution of mercury within OU-2 encompasses the distribution of DDTR and HCB, as shown in the RI Addendum (AMEC, 2011b). Addressing risk associated with mercury concentrations will also address risk associated with DDTR and HCB concentrations.

Recommended Soil PRGs

The recommended mercury cleanup goal for soils is 1.7 mg/kg dw based on risk to the Carolina wren. The recommended mercury PRG of 1.7 mg/kg was calculated using data from crawling insects and spiders.

The recommended soil cleanup goal for DDTR is 3 mg/kg based on upgradient concentrations that are acceptable to EPA and may serve as an ongoing source of DDTR in OU-2. HCB concentrations do not pose unacceptable risk within the floodplain soils, and a HCB PRG was not calculated.

The recommended cleanup goals for soil are listed below.

- Mercury: 1.7 mg/kg
- DDTR: 1 to 3 mg/kg

These PRGs are recommended as remedial goals.

6.0 REFERENCES

Allison, J.D. and T.L. Allison, 2005. *Partition Coefficients for Metals in Surface Water, Soil, and Waste.* EPA/600/R-05/074. July 2005.

AMEC, 2011a. *Part 1: Remedial Investigation Addendum and Enhanced Sedimentation Pilot Project Annual Report—Year Two Results.* Operable Unit 2, Olin Corporation, McIntosh, Alabama. November 14, 2011.

AMEC, 2011b. *Part 2: Updated Ecological Risk Assessment.* Operable Unit 2, Olin Corporation, McIntosh, Alabama. November 14, 2011.

Burkhard, L. 2009. *Estimation of Biota Sediment Accumulation Factor (BSAF) from Paired Observations of Chemical Concentrations in Biota and Sediment*. U.S. Environmental Protection Agency, Ecological Risk Assessment Support Center, Cincinnati, OH. EPA/600/R-06/047.

Gilbert, R.O., 1987. *Statistical Methods for Environmental Pollution Monitoring.* Van Nostrand Reinhold, New York, New York. ISBN 0-442-23050-8.

ProUCL, V4.0. *ProUCL Version 4.00.02 User Guide.* EPA/600/R-07/038. Authors A. Singh, Ph.D., R. Maichle, A.K. Singh, Ph.D., S.E. Lee, and N. Armbya. Editor J. Nocerino. U.S. Environmental Protection Agency, Office of Research and Development, National Exposure Research Laboratory, Environmental Sciences Division, Characterization and Monitoring Branch, Las Vegas, Nevada. April 2007.

Ryan, Sandra E and Laurie Porth, 2007. A Tutorial on the Piecewise Regression Approach Applied to Bedload Transport Data. Gen. Tech. Report. RMRS-GTR-189. Fort Collins, CO: U.S. Department of Agriculture, Forest Service, Rocky Mountain Research Station.

USEPA, 1993. *Wildlife Exposure Factors Handbook Volume II.* United States Environmental Protection Agency, Office of Research and Development, EPA/600/R-93/187b, December 1993.

USEPA, 2010. *SERAFM—Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury.* http://www.epa.gov/ceampubl/swater/serafm/index.html.

URS, 2002. *OU2 RGO Support Sampling Report.* McIntosh Plant Site, Olin Corporation, McIntosh, Alabama. April 15, 2002.

WCC, 1993. *Remedial Investigation Report.* McIntosh Plant Site, Olin Corporation, McIntosh, Alabama. February 1993.

TABLES

TABLE 2-1

Summary of Equations for Mercury in Predatory Fish
OLIN McINTOSH OU-2

	Number of Data Pairs (a)	R^2	Regression Equation (b)	p-value
Largemouth Bass - Power				
1991, 1994	3	0.80	$y = 0.3129x^{0.2529}$	0.003
2001	2	0.82	$y = 0.3814x^{0.3057}$	0.01
2008	4	0.91	$y = 0.4254x^{0.3535}$	0.0002
Years Combined	9	0.85	$y = 0.3642x^{0.3307}$	2E-06
Largemouth Bass - Ratio				
Years Combined	9	NA	$y = 0.0441x$	NA
Largemouth Bass - Linear				
1991, 1994	3	0.89	$y = 0.0186x + 0.2154$	0.0005
2001	2	0.92	$y = 0.0413x + 0.1859$	0.002
2008	4	0.94	$y = 0.0368x + 0.2297$	8E-05
Years Combined	9	0.77	$y = 0.0309x + 0.2459$	4E-05

Notes:

(a) Number of data pairs does not include the five reference area data pairs; Only data pairs for sediments < 45 mg/kg are included in the analysis.

(b) Regression equation based on OU-2 and reference area data pairs.

y = target predatory fish tissue concentration

x = target sediment concentration

NA = Not Applicable

PREPARED BY/DATE: MKB 3/26/12

CHECKED BY/DATE: NSR 3/28/12

TABLE 2-2a

Summary of Equations for Mercury in Forage Fish
OLIN McINTOSH OU-2

	Number of Data Pairs (a)	R^2	Regression Equation (b)	p-value
Power				
Mosquitofish	4	0.90	$y = 0.1414x^{0.3011}$	0.001
Bluegill	4	0.94	$y = 0.1753x^{0.4013}$	0.0003
Silverside	4	0.95	$y = 0.1855x^{0.429}$	0.0002
Species Combined	12	0.87	$y = 0.1646x^{0.3904}$	4E-07
Ratio				
All Forage Fish	12	NA	$y = 0.0236x$	NA
Linear				
Mosquitofish	4	0.96	$y = 0.0135x + 0.0786$	8E-05
Bluegill	4	0.89	$y = 0.0185x + 0.1108$	0.001
Silverside	4	0.94	$y = 0.0224x + 0.1069$	0.0003
Species Combined	12	0.79	$y = 0.0197x + 0.0866$	1E-05

Notes:
(a) Number of data pairs does not include the three reference area data pairs; Only data pairs for sediments < 45 mg/kg are included in the analysis.
(b) Regression equation based on OU-2 and reference area data pairs.
y = target predatory fish tissue concentration
x = target sediment concentration
NA = Not Applicable

PREPARED BY/DATE: MKB 3/26/12
CHECKED BY/DATE: NSR 3/28/12

TABLE 2-2b

Calculation of Sediment-Fish Tissue Ratios - Mercury
OLIN McINTOSH OU-2

Media	Average Fish Tissue Concentration for Mercury (mg/kg)	Average Sediment Concentration for Mercury (mg/kg, dw) (a)	Mercury BSAF (Ratio Method) (b)
Predatory Fish - All Years (c)	0.822	18.6	0.0441
Forage Fish - All Years (d)	0.518167	21.9	0.0236

Notes:
(a) Excludes sediments greater than 45 mg/kg.
(b) BSAF = Average Tissue Concentration/Average Sediment Concentration
(c) Refer to Appendix A, Table A-1 for samples used to calculate the average concentrations.
(d) Refer to Appendix A, Table A-2 for samples used to calculate the average concentrations.
mg/kg = milligrams per kilogram

TABLE 2-3a

Summary of Equations for DDTR in Forage Fish
OLIN McINTOSH OU-2

	Number of Data Pairs (a)	R^2	Regression Equation (b)	p-value
Mosquitofish - Normalized				
Power	9	0.78	$y = 3.4605x^{0.7252}$	0.0001
Ratio	9	NA	$y = 1.08x$	NA
Linear	9	0.68	$y = 0.8019x + 23.813$	0.0009
Mosquitofish - Non-normalized				
Power	9	0.61	$y = 1.2874x^{0.612}$	0.003
Ratio	9	NA	$y = 1.10x$	NA
Linear	9	0.44	$y = 1.1794x - 0.2816$	0.02

Notes:
(a) Number of data pairs does not include the three reference area data pairs.
(b) Regression equation based on OU-2 and reference area data pairs.
y = target predatory fish tissue concentration
x = target sediment concentration
NA = Not Applicable

PREPARED BY/DATE: MKB 3/26/12
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TABLE 2-3b

Calculation of Sediment-Fish Tissue Ratios - DDTR
OLIN McINTOSH OU-2

Media	Average Fish Tissue Concentration for DDTR (mg/kg) (a)	Average Sediment Concentration for DDTR (mg/kg, dw) (a)	DDTR BSAF (Ratio Method) (b)
Normalized Data			
Mosquitofish - All Years	91.8	84.8	1.08
Non-normalized Data			
Mosquitofish - All Years	3.81	3.47	1.10

Notes:
(a) Refer to Appendix A, Table A-3 for samples used to calculate the average concentration.
(b) BAF = Average Tissue Concentration/Average Sediment Concentration
mg/kg = milligrams per kilogram
dw = dry weight

TABLE 2-4

Summary of NOAEL, LOAEL, and Geometric Mean Target Concentrations in Media
OLIN McINTOSH OU-2

Receptor	Hg				MeHg				DDTR				HCB			
	NOAEL Target (mg/kg)	LOAEL Target (mg/kg)	Geometric Mean Target (mg/kg)	Controlling Media	NOAEL Target (mg/kg)	LOAEL Target (mg/kg)	Geometric Mean Target (mg/kg)	Controlling Media	NOAEL Target (mg/kg)	LOAEL Target (mg/kg)	Geometric Mean Target (mg/kg)	Controlling Media	NOAEL Target (mg/kg)	LOAEL Target (mg/kg)	Geometric Mean Target (mg/kg)	Controlling Media
Mink	27	27	27	Sediment	NA	NA	NA	NA	NA	NA	NA	NA	7.6	7.6	7.6	Sediment
Belted Kingfisher (Highly Conservative Scenario)	NA	NA	NA	NA	0.11	0.11	0.11	FF	0.42	0.52	0.47	FF	NA	NA	NA	NA
Belted Kingfisher (Reasonable Maximum Exposure)	NA	NA	NA	NA	0.35	0.35	0.35	FF	0.80	1.19	0.98	FF	NA	NA	NA	NA
Pied Billed Grebe	NA	NA	NA	NA	0.58	0.58	0.58	FF	0.51	1.20	0.78	FF	NA	NA	NA	NA
Little Blue Heron	NA	NA	NA	NA	0.20	0.20	0.20	FF	0.62	0.82	0.71	FF	NA	NA	NA	NA
Great Blue Heron	NA	NA	NA	NA	0.20/0.43[a]	0.20/0.43[a]	0.20/0.43[a]	FF/PF	1.29	1.78[b]	1.52	FF	NA	NA	NA	NA

Notes:

(a) Forage fish concentration assumed to be equal to little blue heron forage fish PRG and then the MeHg PRG for predatory fish was back calculated.

(b) Allowable concentration is above the current site-wide exposure point concentration. Value included to find the geometric mean target concentration.

NOAEL = No Observed Adverse Effects Level

LOAEL = Lowest Observed Adverse Effects Level

NA = Not Applicable. Risk not indicated for this receptor and constituent.

AI = Aquatic Insect

PF = Predatory Fish (Largemouth Bass)

FF = Forage Fish (Bluegill, Silverside, Mosquitofish)

mg/kg = milligrams per kilogram

PREPARED BY/DATE: MKB 3/26/12

CHECKED BY/DATE: NSR 3/28/12

TABLE 2-5

Calculation of Sediment PRGs Based on Target Predatory Fish Concentrations - Mercury
OLIN McINTOSH OU-2

	Allowed Predatory Fish Tissue Concentration [a] for Mercury (mg/kg) (y)	Equation	R^2	p-value	Target Sediment Concentration for Mercury (mg/kg) (x)
	NOAEL/LOAEL/GEOMEAN [b]				NOAEL/LOAEL/GEOMEAN [b]
Power Analysis					
1991, 1994	0.43	$y = 0.3129x^{0.2529}$	0.80	0.003	3.5
2001	0.43	$y = 0.3814x^{0.3057}$	0.82	0.01	1.5
2008	0.43	$y = 0.4254x^{0.3535}$	0.91	0.0002	1.0
Years Combined	0.43	$y = 0.3642x^{0.3307}$	0.85	2E-06	1.7
Ratio					
Years Combined	0.43	y = 0.0441x	NA	NA	9.8
Linear Analysis					
1991, 1994	0.43	y = 0.0186x + 0.2154	0.89	0.0005	12
2001	0.43	y = 0.0413x + 0.1859	0.92	0.002	5.9
2008	0.43	y = 0.0368x + 0.2297	0.94	8E-05	5.4
Years Combined	0.43	y = 0.0309x + 0.2459	0.77	4E-05	6.0

Notes:
(a) The great blue heron is the only ecological receptor with predatory fish as a controlling media (Table 2-4).
(b) As shown on Table 2-4, the NOAEL and LOAEL target predatory fish concentrations are the same, resulting in the same concentration for the geometric mean concentration.
y = allowed largemouth bass fish tissue concentration
x = target sediment concentration associated with allowed fish concentration
mg/kg = milligrams per kilogram
PRG = Preliminary Remediation Goal
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level
GEOMEAN = Geometric mean of the NOAEL and LOAEL

Indicates the equation that provides the highest R^2 value with an acceptable p-value (<0.05).

Indicates the combined equation considered representative of a more robust dataset, as demonstrated by the increased sample size and lower p-value, than the year-specific regression lines; equation achieves USEPA's goals of statistical relevance (R^2 value > 0.70 and a p-value < 0.05).

PREPARED BY/DATE: NSR 5/21/12
CHECKED BY/DATE: EFC 5/21/12

TABLE 2-6

Calculation of Sediment PRGs Based on Target Forage Fish Concentrations - Mercury
OLIN McINTOSH OU-2

		Allowed Forage Fish Tissue Concentration[a] for Mercury (mg/kg) (y)	Equation	R^2	p-value	Target Sediment Concentration for Mercury (mg/kg) (x)
		NOAEL/LOAEL/GEOMEAN[b]				NOAEL/LOAEL/GEOMEAN[b]
Belted Kingfisher (Highly Conservative Scenario)						
Mosquitofish	Power Analysis	0.11	$y = 0.1414x^{0.3011}$	0.90	0.001	0.43
Bluegill	Power Analysis	0.11	$y = 0.1753x^{0.4013}$	0.94	0.0003	0.31
Silverside	Power Analysis	0.11	$y = 0.1855x^{0.429}$	0.95	0.0002	0.30
Species Combined	Power Analysis	0.11	$y = 0.1646x^{0.3904}$	0.87	4E-07	0.36
Species Combined	Ratio	0.11	y = 0.0236x	NA	NA	4.7
Mosquitofish	Linear Analysis	0.11	y = 0.0135x + 0.0786	0.96	8E-05	2.3
Bluegill	Linear Analysis	0.11	y = 0.0185x + 0.1108	0.89	0.001	-0.043
Silverside	Linear Analysis	0.11	y = 0.0224x + 0.1069	0.94	0.0003	0.14
Species Combined	Linear Analysis	0.11	y = 0.0197x + 0.0866	0.79	1E-05	1.2
Belted Kingfisher (Reasonable Maximum Exposure)						
Mosquitofish	Power Analysis	0.35	$y = 0.1414x^{0.3011}$	0.90	0.001	20
Bluegill	Power Analysis	0.35	$y = 0.1753x^{0.4013}$	0.94	0.0003	5.6
Silverside	Power Analysis	0.35	$y = 0.1855x^{0.429}$	0.95	0.0002	4.4
Species Combined	Power Analysis	0.35	$y = 0.1646x^{0.3904}$	0.87	4E-07	6.9
Species Combined	Ratio	0.35	y = 0.0236x	NA	NA	15
Mosquitofish	Linear Analysis	0.35	y = 0.0135x + 0.0786	0.96	8E-05	20
Bluegill	Linear Analysis	0.35	y = 0.0185x + 0.1108	0.89	0.001	13
Silverside	Linear Analysis	0.35	y = 0.0224x + 0.1069	0.94	0.0003	11
Species Combined	Linear Analysis	0.35	y = 0.0197x + 0.0866	0.79	1E-05	13
Pied Billed Grebe						
Mosquitofish	Power Analysis	0.58	$y = 0.1414x^{0.3011}$	0.90	0.001	109
Bluegill	Power Analysis	0.58	$y = 0.1753x^{0.4013}$	0.94	0.0003	20
Silverside	Power Analysis	0.58	$y = 0.1855x^{0.429}$	0.95	0.0002	14
Species Combined	Power Analysis	0.58	$y = 0.1646x^{0.3904}$	0.87	4E-07	25
Species Combined	Ratio	0.58	y = 0.0236x	NA	NA	25
Mosquitofish	Linear Analysis	0.58	y = 0.0135x + 0.0786	0.96	8E-05	37
Bluegill	Linear Analysis	0.58	y = 0.0185x + 0.1108	0.89	0.001	25
Silverside	Linear Analysis	0.58	y = 0.0224x + 0.1069	0.94	0.0003	21
Species Combined	Linear Analysis	0.58	y = 0.0197x + 0.0866	0.79	1E-05	25

TABLE 2-6

Calculation of Sediment PRGs Based on Target Forage Fish Concentrations - Mercury
OLIN McINTOSH OU-2

		Allowed Forage Fish Tissue Concentration[a] for Mercury (mg/kg) (y)	Equation	R^2	p-value	Target Sediment Concentration for Mercury (mg/kg) (x)
		NOAEL/LOAEL/GEOMEAN[b]				NOAEL/LOAEL/GEOMEAN[b]
Little Blue Heron						
Mosquitofish	Power Analysis	0.20	$y = 0.1414x^{0.3011}$	0.90	0.001	3.2
Bluegill	Power Analysis	0.20	$y = 0.1753x^{0.4013}$	0.94	0.0003	1.4
Silverside	Power Analysis	0.20	$y = 0.1855x^{0.429}$	0.95	0.0002	1.2
Species Combined	Power Analysis	0.20	$y = 0.1646x^{0.3904}$	0.87	4E-07	1.6
Species Combined	Ratio	0.20	$y = 0.0236x$	NA	NA	8.5
Mosquitofish	Linear Analysis	0.20	$y = 0.0135x + 0.0786$	0.96	8E-05	9.0
Bluegill	Linear Analysis	0.20	$y = 0.0185x + 0.1108$	0.89	0.001	4.8
Silverside	Linear Analysis	0.20	$y = 0.0224x + 0.1069$	0.94	0.0003	4.2
Species Combined	Linear Analysis	0.20	$y = 0.0197x + 0.0866$	0.79	1E-05	5.8

Notes:
(a) Table 2-4
(b) As shown on Table 2-4, the NOAEL and LOAEL target forage fish concentrations are the same, resulting in the same concentration for the geometric mean concentration.
y = allowed forage fish tissue concentration
x = target sediment concentration associated with allowed fish concentration
mg/kg = milligrams per kilogram
PRG = Preliminary Remediation Goal
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level
GEOMEAN = Geometric mean of the NOAEL and LOAEL

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Indicates the equation that provides the highest R^2 value with an acceptable p-value (<0.05).

Indicates the combined equation considered representative of a more robust dataset, as demonstrated by the increased sample size and lower p-value, than the species-specific regression lines; equation achieves USEPA's goals of statistical relevance (R^2value > 0.70 and a p-value < 0.05).

TABLE 2-7

Calculation of Sediment PRGs Based on Target Forage Fish Concentrations - DDTR (Normalized)
OLIN McINTOSH OU-2

		Allowed Forage Fish Tissue Concentration for DDTR [a] (mg/kg) (y)			Allowed Forage Fish Tissue Concentration for DDTR [b] (Normalized) (mg/kg) (y)			Normalized Equation	R^2	p-value	Target Sediment Concentration for DDTR (Normalized) (mg/kg) (x)			Target Sediment Concentration for DDTR [c] (mg/kg) (x)		
		NOAEL	LOAEL	GEOMEAN	NOAEL	LOAEL	GEOMEAN				NOAEL	LOAEL	GEOMEAN	NOAEL	LOAEL	GEOMEAN
Belted Kingfisher (Highly Conservative Scenario)																
Mosquitofish	Power Analysis	0.42	0.52	0.47	11	14	13	$y = 3.4605x^{0.7252}$	0.78	0.0001	5.15	6.91	6.01	0.28	0.38	0.33
Belted Kingfisher (Reasonable Maximum Exposure)																
Mosquitofish	Power Analysis	0.80	1.19	0.98	22	32	26	$y = 3.4605x^{0.7252}$	0.78	0.0001	12.51	21.63	16.55	0.69	1.19	0.91
Pied Billed Grebe																
Mosquitofish	Power Analysis	0.51	1.20	0.78	14	32	21	$y = 3.4605x^{0.7252}$	0.78	0.0001	6.72	21.88	12.08	0.37	1.20	0.66
Little Blue Heron																
Mosquitofish	Power Analysis	0.62	0.82	0.71	17	22	19	$y = 3.4605x^{0.7252}$	0.78	0.0001	8.80	12.94	10.61	0.48	0.71	0.58
Great Blue Heron																
Mosquitofish	Power Analysis	1.29	1.78	1.52	35	48	41	$y = 3.4605x^{0.7252}$	0.78	0.0001	24.18	37.69	30.32	1.33	2.07	1.67

Notes:
(a) Table 2-4
(b) Fish tissue normalized by dividing allowed tissue concentration by the average fraction lipids (0.037) in mosquitofish samples.
(c) Target sediment concentration denormalized by multiplying by the average fraction of organic carbon (0.055) in sediment samples.
y = allowed forage fish tissue concentration
x = target sediment concentration associated with allowed fish concentration
mg/kg = milligrams per kilogram
PRG = Preliminary Remediation Goal
NA = Not Applicable
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level
GEOMEAN = Geometric mean of the NOAEL and LOAEL
Indicates the equation that provides the highest R^2 value with an acceptable p-value (<0.05).

PREPARED BY/DATE: MKB 3/26/12
CHECKED BY/DATE: NSR 3/28/12

TABLE 2-8

Summary of Mercury PRGs for Sediment - Based on Risk from Predatory Fish
OLIN McINTOSH OU-2

Receptor	Range of Target Sediment Concentrations Protective of Receptor (mg/kg)								
	Power Analysis	R^2	p-value	Ratio (a)	R^2	p-value	Linear	R^2	p-value
Great Blue Heron	**NOAEL/LOAEL/GEOMEAN**			**NOAEL/LOAEL/GEOMEAN**			**NOAEL/LOAEL/GEOMEAN**		
1991, 1994	3.5	0.80	0.003	NA	NA	NA	12	0.89	0.0005
2001	1.5	0.82	0.01	NA	NA	NA	5.9	0.92	0.002
2008	1.0	0.91	0.0002	NA	NA	NA	5.4	0.94	8E-05
Years Combined	1.7	0.85	2E-06	9.8	NA	NA	6.0	0.77	4E-05
OVERALL RANGE	**1.0 - 3.5**			**9.8**			**5.4 - 12**		

RANGE OF MERCURY SEDIMENT PRGs (mg/kg) (Across All Types of Analysis)	**1.0 - 12**

Notes:

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(a) Ratio method presented for information purposes only and not included in the overall range.
PRG = Preliminary Remediation Goal
mg/kg = milligrams per kilogram
NA = Not Applicable
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level

GEOMEAN = Geometric mean of the NOAEL and LOAEL

Indicates the PRG calculated using the equation that provides the highest R^2 with an acceptable p-value (<0.05).

Indicates the PRG calculated using the equation considered representative of a more robust dataset, as demonstrated by the increased sample size and lower p-value, than the year-specific regression lines; equation achieves USEPA's goals of statistical relevance (R^2 value > 0.70 and a p-value < 0.05).

TABLE 2-9

Summary of Mercury PRGs for Sediment - Based on Risk from Forage Fish
OLIN McINTOSH OU-2

Receptor	Range of Target Sediment Concentrations Protective of Receptor (mg/kg)									
	Power Analysis	R^2	p-value	Ratio (a)	R^2	p-value	Linear	R^2	p-value	Overall Range
Belted Kingfisher (Highly Conservative Scenario)	**NOAEL/LOAEL/GEOMEAN**			**NOAEL/LOAEL/GEOMEAN**			**NOAEL/LOAEL/GEOMEAN**			
Mosquitofish	0.43	0.90	0.001	NA	NA	NA	2.3	0.96	8E-05	
Bluegill	0.31	0.94	0.0003	NA	NA	NA	-0.043	0.89	0.001	
Silverside	0.30	0.95	0.0002	NA	NA	NA	0.14	0.94	0.0003	
Species Combined	0.36	0.87	4E-07	4.7	NA	NA	1.2	0.79	1E-05	
OVERALL RANGE	**0.30 - 0.43**			**4.7**			**-0.043 - 2.3**			**-0.043 - 2.3**
Belted Kingfisher (Reasonable Maximum Exposure)										
Mosquitofish	20	0.90	0.001	NA	NA	NA	20	0.96	8E-05	
Bluegill	5.6	0.94	0.0003	NA	NA	NA	13	0.89	0.001	
Silverside	4.4	0.95	0.0002	NA	NA	NA	11	0.94	0.0003	
Species Combined	6.9	0.87	4E-07	15	NA	NA	13	0.79	1E-05	
OVERALL RANGE	**4.4 - 20**			**15**			**11-20**			**4.4 - 20**
Pied Billed Grebe										
Mosquitofish	109	0.90	0.001	NA	NA	NA	37	0.96	8E-05	
Bluegill	20	0.94	0.0003	NA	NA	NA	25	0.89	0.001	
Silverside	14	0.95	0.0002	NA	NA	NA	21	0.94	0.0003	
Species Combined	25	0.87	4E-07	25	NA	NA	25	0.79	1E-05	
OVERALL RANGE	**14 - 109**			**25**			**21 - 37**			**14 - 109**
Little Blue Heron										
Mosquitofish	3.2	0.90	0.001	NA	NA	NA	9.0	0.96	8E-05	
Bluegill	1.4	0.94	0.0003	NA	NA	NA	4.8	0.89	0.001	
Silverside	1.2	0.95	0.0002	NA	NA	NA	4.2	0.94	0.0003	
Species Combined	1.6	0.87	4E-07	8.5	NA	NA	5.8	0.79	1E-05	
OVERALL RANGE	**1.2 - 3.2**			**8.5**			**4.2 - 9.0**			**1.2 - 9.0**
							RANGE OF MERCURY SEDIMENT PRGs (mg/kg) (Across All Types of Analysis)			**-0.043 - 109**

Notes:
(a) Ratio method presented for information purposes only and not included in the overall range.
PRG = Preliminary Remediation Goal
mg/kg = milligrams per kilogram
NA = Not Applicable
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level
GEOMEAN = Geometric mean of the NOAEL and LOAEL

Indicates the PRG calculated using the equation that provides the highest R^2 with an acceptable p-value (<0.05).

Indicates the PRG calculated using the equation considered representative of a more robust dataset, as demonstrated by the increased sample size and lower p-value, than the species-specific regression lines; equation achieves USEPA's goals of statistical relevance (R^2 value > 0.70 and a p-value < 0.05).

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TABLE 2-10

Summary of DDTR PRGs for Sediment - Based on Risk from Forage Fish
OLIN McINTOSH OU-2

Receptor	Range of Target Sediment Concentrations Protective of Receptor (mg/kg)					
	Power			R^2	p-value	Overall Range
	NOAEL	LOAEL	GEOMEAN			
Normalized Data						
Belted Kingfisher (Highly Conservative Scenario)						
Mosquitofish	0.28	0.38	0.33	0.78	0.0001	0.28 - 0.38
Belted Kingfisher (Reasonable Maximum Exposure)						
Mosquitofish	0.69	1.2	0.91	0.78	0.0001	0.69 - 1.2
Pied Billed Grebe						
Mosquitofish	0.37	1.2	0.66	0.78	0.0001	0.37 - 1.2
Little Blue Heron						
Mosquitofish	0.48	0.71	0.58	0.78	0.0001	0.48 - 0.71
Great Blue Heron						
Mosquitofish	1.3	2.1	1.7	0.78	0.0001	1.3 - 2.1
					RANGE OF DDTR SEDIMENT PRGs (mg/kg) (Across All Types of Analysis)	**0.28 - 2.1**

Notes:
PRG = Preliminary Remediation Goal
mg/kg = milligrams per kilogram
NA = Not Applicable
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level
GEOMEAN = Geometric mean of the NOAEL and LOAEL

Indicates the PRG calculated using the equation that provides the highest R^2 with an acceptable p-value (<0.05).

PREPARED BY/DATE: MKB 3/26/12
CHECKED BY/DATE: NSR 3/28/12

TABLE 3-1

SERAFM Input Parameters and Justification for Selection
OLIN McINTOSH OU-2

Parameter	Scenario 1 6 ft Water Elevation		Scenario 2 3 ft Water Elevation		Justification for Selection
	Input Set 1	Input Set 2	Input Set 1	Input Set 2	
Analytical Data Source Year(s)	2009		2008 and 2009		Years from which analytical data are used for inputs; 2009 porewater data used in 2008 scenarios because it is the closest dataset temporally to 2008.
Water Elevation Basis (ft NAVD88)	6		3		Water elevation basis used to determine area and other hydraulic parameters.
Lake Area (m^2)	275,681		274,544		Based on indicated elevation, area of Basin and Round Pond, excluding the area of the Deep Hole[1].
Watershed Area, as Contributing Area (m^2)	647,500		647,500		OU-2 watershed area east of the bluff and inside the berm under non-flood conditions.
Epilimnion Depth (m)	1.4		0.49		Calculated from July and August 2009 temperature profiles.
Hypolimnion Depth (m)	0.1		0.1		SERAFM minimum value. This model represents the epilimnion only.
Anoxic Hypolimnion?	Yes		Yes		Based on July and August 2009 dissolved oxygen profiles.
Inflow (m^3/yr)	6.80E+06		3.47E+06		Steady state assumption (inflow = outflow); an average of the inflow and outflow for the year was computed from water level data. See Appendix C.
Outflow (m^3/yr)	6.80E+06		3.47E+06		Steady state assumption (inflow = outflow); an average of the inflow and outflow for the year was computed from water level data. See Appendix C.
Precipitation (centimeters per year)	152.40		105.20		Scenario 1 uses 2009 total precipitation data. Scenario 2 uses 2008 total precipitation data. Scenario 3 is based on summer 2008 rainfall, extrapolated out to a year.
DOC Epilimnion (mg/L)	16		17		Average DOC concentration of indicated year(s) SW ESPP monitoring samples collected in epiliminon (excludes samples in Deep Hole[1]).
DOC Hypolimnion (mg/L)	16		17		Same as above - model represents epilimnion only.
HgII - River (g/m^3)	5.64E-06		5.64E-06		Average of 2 Tombigbee River samples collected on 11/02/2009 (2008 data not available).
Hg conc. in sed dry weight (µg/g)	33.27		40.7		Average of 2009 0-2" fine sediment cores and indicated year(s) 0-4" surficial sediment samples. Excludes samples taken in the Deep Hole[1].
Zooplankton biotic solids in water inflow (g/m^3)	1	5	1	5	Input Set 1: Default model input for eutrophic lake; Input Set 2: Suggested value from model author for eutrophic lake
Process/Media					
Methylation/Sediment (per day)	1.60E-07		1.60E-07		Adjusted for calibration.
Demethylation/Hypolimnion (per day)	1.60E-07		1.60E-07		Adjusted for calibration.
Demethylation/Sediment (per day)	3.20E-07		3.20E-07		Adjusted for calibration.
Photodegradation/Water Column (per day E/m^2-day)	2.00E-03		2.00E-03		Adjusted for calibration.
HgII K_d_sed (L/kg)	260,558		260,558		From Battelle data as interpreted by AMEC using a log-log regression point Kd estimate
MeHg K_d_sed (L/kg)	4,557		4,557		From Battelle data as interpreted by AMEC using a log-log regression point Kd estimate
HgII Kd_abio (L/kg)	7,182,936		7,182,936		Input Set 1: Ratio of abio to bio is ; Input Set 2: ratio of abio to bio is 2.5
HgII Kd_bio (L/kg)	127,696,640	17,941,378	127,696,640	17,941,378	
Particle Parameters					
Abiotic solids in water inflow (g/m^3)	44		44		From Anchor QEA analysis provided in Updated RI Addendum (AMEC, 2011a).
Sediment particle diameter (µm)	13		13		Lowest geometric mean of the particle sizes as analyzed from the October 2009 storm event. Particle distribution not expected to be notably different between storm events.
Burial velocity (m/yr)	0.008		0.008		From Anchor QEA analysis provided in Updated RI Addendum (AMEC, 2011a).

Notes:

[1]Samples from locations 103, 203 and DH are located in the Deep Hole area, which was excluded from the model.

Grey highlight denotes parameters that were adjusted to calibrate the model.

Methylation/demethylation rates are default value with scaling factors applied for calibration.

Where the same inputs were used for Input Set 1 and Input Set 2, the inputs are listed only once

Prepared by/Date: NTG 4/13/2012
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DOC = dissolved organic carbon
E/m^2-day = Einsteins per square meter per day
g/m^3 = grams per cubic meter
HgII = inorganic mercury
K_d = partition coefficient
L/kg = liter per kilogram
µg/g = microgram per gram
µm = micrometer
m = meter
m/yr = meter per year
m^2 = square meter
m^3/yr = cubic meter per year
MeHg = methylmercury
mg/L = milligram per liter
SW = surface water

TABLE 3-2

SERAFM Calibration and Confirmation Results
OLIN McINTOSH OU-2

INPUT SET 1	MODEL CALIBRATION - SCENARIO 1			MODEL CONFIRMATION - SCENARIO 2		
	Predicted by SERAFM Scenario 1, Input Set 1[1]	Measured in 2009 (Scenario 1)[1]	Percent Difference[2,3,4]	Predicted by SERAFM Scenario 2, Input Set 1[1]	Measured in 2008 (Scenario 2)[1]	Percent Difference[2,3,4]
Epilimnion Surface Water						
Filtered Methylmercury (µg/L)	0.000460	0.000475	3.27%	0.000750	0.000770	2.67%
Filtered Mercury (µg/L)	0.0191	0.00739	-61.3%	0.0228	0.0153	-33.1%
Unfiltered Methylmercury (µg/L)	0.000890	0.000882	-0.87%	0.00142	0.00278	95.8%
Unfiltered Mercury (µg/L)	0.105	0.0427	-59.4%	0.0931	0.266	186%
		Average Percent Difference	-29.6%		Average Percent Difference	62.8%
		Average Absolute Percent Difference	31.2%		Average Absolute Percent Difference	79.6%

INPUT SET 2	MODEL CALIBRATION - SCENARIO 1			MODEL CONFIRMATION - SCENARIO 2		
	Predicted by SERAFM Scenario 1, Input Set 2[1]	Measured in 2009 (Scenario 1)[1]	Percent Difference[2,3,4]	Predicted by SERAFM Scenario 2, Input Set 2[1]	Measured in 2008 (Scenario 2)[1]	Percent Difference[2,3,4]
Epilimnion Surface Water						
Filtered Methylmercury (µg/L)	0.000434	0.000475	9.50%	0.000743	0.000770	3.65%
Filtered Mercury (µg/L)	0.0153	0.00739	-51.7%	0.0193	0.0153	-20.9%
Unfiltered Methylmercury (µg/L)	0.00247	0.000882	-64.3%	0.00406	0.00278	-31.5%
Unfiltered Mercury (µg/L)	0.0803	0.0427	-46.9%	0.0773	0.266	244%
		Average Percent Difference	-38.3%		Average Percent Difference	48.9%
		Average Absolute Percent Difference	43.1%		Average Absolute Percent Difference	75.1%

Notes:

[1]Sources of inputs and measured values used are listed in Table 3-1

[2]Percent Difference calculated as (measured - predicted) ÷ predicted

[3]Negative Percent Difference indicates that model overpredicts result

[4] Average Absolute Percent Difference calculated as (|measured - predicted|) ÷ predicted

Order of preference for calibration/confirmation per USEPA model developer: 1) filtered methylmercury, 2) filtered mercury, 3) unfiltered methylmercury, 4) unfiltered mercury.

µg/L = micrograms per liter

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Checked by/Date: KPW 04/17/2012

TABLE 3-3

SERAFM Target Sediment Mercury Concentrations
Associated with Receptor Hazard Indices of 1
OLIN McINTOSH OU-2

Ecological Receptor	Target Sediment Mercury concentration, dry weight (mg/kg)
	Scenario 1
Belted Kingfisher - 100% TL3 Fish, FF = 1	4.2 - 7.4
Belted Kingfisher - Modified Diet*, FF = 0.5	14.8 - 17.6
Little Blue Heron	10.7 - 13.6
Great Blue Heron	13.1 - 16.0
Mink	30.6 - 32.7
Pied-billed Grebe	33.9 -35.9

Notes:
FF = Forage Factor
Scenario defined in Table 3-1; Given range represents both Input Set 1 and Input Set 2
mg/kg = milligrams per kilogram
TL = trophic level
*frogs 35%, TL3 fish 45%, TL4 fish 20%

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Checked by/Date: KPW 04/17/2012

TABLE 3-4a

SERAFM Sensitivity Analysis for the Little Blue Heron Using Scenario 1, Input Set 1 [1]
OLIN McINTOSH OU-2

	Input			Variability From Base Target Sediment Concentration of 10.7 mg/kg dw	
	80% of Scenario 1	Scenario 1	120% of Scenario 1		
Lake Area[2] (m^2)	417,029 [2]	463,365	509,702 [2]	4.9%	-4.0%
Epilimnion Depth (m)	1.1	1.4	1.7	-2.0%	1.6%
Inflow (m^3/yr)	5,437,372	6,796,715	8,156,058	3.5%	-3.5%
precipitation (in/yr)	48	60	72	3.8%	-3.8%
DOC Epilimnion (mg/L)	12.8	16.0	19.2	15.2%	-10.8%
DOC Hypolimnion (mg/L)	12.8	16.0	19.2	0.0%	0.0%
HgII - River (g/m^3)	0.00000451	0.00000564	0.00000677	3.5%	-3.5%
Hg conc. in sed dry weight (µg/g)	26.6	33.3	39.9	0.0%	0.0%
HgII K_d_sed (L/kg)[3]	26,056 [3]	260,558	2,605,580 [3]	0.0%	0.0%
MeHg K_d_sed (L/kg)[3]	456 [3]	4,557	45,570 [3]	0.0%	0.0%
Abiotic solids in water inflow (g/m^3)	35	44	53	0.0%	0.0%
Sediment particle diameter (µm)[4]	7	13	24	0.1%	0.0%
Burial velocity (m/yr)	0.006	0.008	0.009	0.0%	0.0%

Notes:

Prepared/Date: KPW 04/17/2012

Checked/Date: NTG 04/17/2012

[1]Scenario 1, Input Set 1 input values and sources used are listed in Table 3-1.

[2]Lake Area was varied from 90% to 110% for sensitivity analysis.

[3]Adsorption Coefficients for mercury and methylmercury in sediment were varied by factors of 0.1 and 10.

[4]Sediment particle size was varied based on the range of geometric means of particle size.

m^2 = meters squared
m = meters
m^3/yr = cubic meters per year
in/yr = inches per year
mg/L = milligrams per liter
g/m^3 = grams per cubic meter
µg/g = microgram per gram
HgII = Mercury (II)
MeHg = Methylmercury
Kd_sed = solid-liquid partition coefficient
L/kg = liters per kilogram
µm = micrometer
m/yr = meters per year
DOC = dissolved organic carbon

TABLE 3-4b

SERAFM Sensitivity Analysis for the Little Blue Heron Using Scenario 1, Input Set 2[1]
OLIN McINTOSH OU-2

	Input			Variability From Base Target Sediment Concentration of 13.61 mg/kg dw	
	80% of Scenario 1	Scenario 1	120% of Scenario 1		
Lake Area[2] (m^2)	417,029 [2]	463,365	509,702 [2]	6.2%	-5.1%
Epilimnion Depth (m)	1.1	1.4	1.7	-2.0%	1.7%
Inflow (m^3/yr)	5,437,372	6,796,715	8,156,058	0.9%	-0.9%
precipitation (in/yr)	48	60	72	1.0%	-1.0%
DOC Epilimnion (mg/L)	12.8	16.0	19.2	18.7%	-13.4%
DOC Hypolimnion (mg/L)	12.8	16.0	19.2	0.1%	0.0%
HgII - River (g/m^3)	0.00000451	0.00000564	0.00000677	0.9%	-0.9%
Hg conc. in sed dry weight (µg/g)	26.6	33.3	39.9	0.0%	0.0%
HgII K_d_sed (L/kg)[3]	26,056 [3]	260,558	2,605,580 [3]	0.0%	0.0%
MeHg K_d_sed (L/kg)[3]	456 [3]	4,557	45,570 [3]	0.0%	0.0%
Abiotic solids in water inflow (g/m^3)	35	44	53	0.0%	0.0%
Sediment particle diameter (µm)[4]	7	13	24	0.0%	0.0%
Burial velocity (m/yr)	0.006	0.008	0.009	0.0%	0.0%

Notes:

Prepared/Date: NTG 04/13/2012

Checked/Date: KPW 04/17/2012

[1]Scenario 1, Input Set 2 input values and sources used are listed in Table 3-1.

[2]Lake Area was varied from 90% to 110% for sensitivity analysis.

[3]Adsorption Coefficients for mercury and methylmercury in sediment were varied by factors of 0.1 and 10.

[4]Sediment particle size was varied based on the range of geometric means of particle size.

m^2 = meters squared
m = meters
m^3/yr = cubic meters per year
in/yr = inches per year
mg/L = milligrams per liter
g/m^3 = grams per cubic meter
µg/g = microgram per gram
HgII = Mercury (II)
MeHg = Methylmercury
Kd_sed = solid-liquid partition coefficient
L/kg = liters per kilogram
µm = micrometer
m/yr = meters per year
DOC = dissolved organic carbon

TABLE 4-1a

Summary of Regression Analysis in Invertebrates Paired with Floodplain Soil
OLIN McINTOSH OU-2

Parameter	Number of Data Pairs	Power Regression Equation	R^2	p-value	Linear Regression Equation	R^2	p-value	Ratio	R^2	p-value
Flying Insects, Crawling Insects, and Spiders										
Mercury, 1994 Included	14	$y = 0.0629x^{-0.292}$	0.043	0.5	y = -0.0154x + 0.1182	0.031	0.5	y = 0.069x	NA	NA
Mercury, 1994 Excluded	13	$y = 0.0607x^{-0.375}$	0.057	0.4	y = -0.0178x + 0.1207	0.022	0.6	y = 0.081	NA	NA
DDTR (normalized), 1994 Included	11	$y = 3.1888x^{0.3221}$	0.11	0.3	y = -0.0499x + 6.4881	0.0056	0.8	y = 1.46x	NA	NA
DDTR (non-normalized), 1994 Included	11	$y = 0.3314x^{0.3374}$	0.22	0.1	y = -0.0089x + 0.2245	0.00035	1.0	y = 1.01x	NA	NA
DDTR (normalized), 1994 Excluded	10	$y = 3.0915x^{0.9136}$	0.33	0.08	y = 4.2354x - 0.2285	0.53	0.02	y = 4.09x	NA	NA
DDTR (non-normalized), 1994 Excluded	10	$y = 0.6485x^{0.5297}$	0.35	0.07	y = 1.5884x + 0.0724	0.47	0.03	y = 2.31x	NA	NA
Spiders										
Mercury	3	$y = 0.0708x^{-0.165}$	0.49	0.5	y = -0.0107x + 0.0831	0.42	0.6	y = 0.060x	NA	NA
DDTR (normalized)	2	NA	NA	NA	NA	NA	NA	NA	NA	NA
DDTR (non-normalized)	2	NA	NA	NA	NA	NA	NA	NA	NA	NA
Flying Insects										
Mercury	5	$y = 0.1399x^{-0.078}$	0.021	0.8	y = -0.0018x + 0.1656	0.00027	1.0	y = 0.14x	NA	NA
DDTR (normalized)	4	$y = 5.9844x^{0.7376}$	0.89	0.06	y = 4.7889x + 0.474	0.83	0.09	y = 5.03x	NA	NA
DDTR (non-normalized)	4	$y = 1.0305x^{0.4174}$	0.92	0.04	y = 2.233x + 0.1313	0.89	0.05	y = 3.58x	NA	NA
Crawling Insects										
Mercury	5	$y = 0.0257x^{-0.388}$	0.024	0.8	y = -0.0259x + 0.0855	0.077	0.7	y = 0.039x	NA	NA
DDTR (normalized)	4	$y = 1.3884x^{0.7811}$	0.19	0.6	y = 0.4519x + 2.6973	0.0054	0.9	y = 2.53x	NA	NA
DDTR (non-normalized)	4	$y = 0.3673x^{0.6763}$	0.64	0.2	y = 1.2273x - 0.0183	0.55	0.3	y = 1.05x	NA	NA
Crawling Insects & Spiders										
Mercury	8	$y = 0.0378x^{-0.398}$	0.030	0.7	y = -0.024x + 0.0889	0.083	0.5	y = 0.046x	NA	NA
DDTR (normalized)	6	$y = 2.0679x^{0.933}$	0.24	0.3	y =1.9769x + 1.7104	0.12	0.5	y = 3.21x	NA	NA
DDTR (non-normalized)	6	$y = 0.5281x^{0.6426}$	0.47	0.1	y = 1.2027x + 0.0304	0.49	0.1	y = 1.50x	NA	NA

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TABLE 4-1b

Calculation of Soil-Soil Invertebrate Ratio - Mercury
OLIN McINTOSH OU-2

Media	Average Invertebrate Tissue Concentration for Methylmercury (mg/kg) (a)	Average Soil Concentration for Mercury (mg/kg, dw) (a)	Mercury BAF (Ratio Method) (b)
Flying Insects, Crawling Insects, and Spiders			
1994 Included	0.097	1.40	0.069
1994 Excluded	0.099	1.22	0.081
Spiders	0.071	1.18	0.060
Flying Insects	0.16	1.15	0.14
Crawling Insects	0.051	1.32	0.039
Crawling Insects & Spiders	0.058	1.27	0.046

Notes:
(a) Refer to Appendix D, Table D-1 for samples used to calculate the average concentration.
(b) BAF = Average Tissue Concentration/Average Soil Concentration
mg/kg = milligrams per kilogram
dw = dry weight

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TABLE 4-1c

Calculation of Soil-Soil Invertebrate Ratio - DDTR
OLIN McINTOSH OU-2

Media	Average Invertebrate Tissue Concentration for DDTR (mg/kg) (a)	Average Soil Concentration for DDTR (mg/kg, dw) (a)	DDTR BAF (Ratio Method) (b)
Normalized Data			
Flying Insects, Crawling Insects, and Spiders			
1994 Included	6.27	4.29	1.46
1994 Excluded	6.56	1.60	4.09
Flying Insects	9.73	1.93	5.03
Crawling Insects	3.28	1.30	2.53
Crawling Insects & Spiders	4.44	1.38	3.21
Non-normalized Data			
Flying Insects, Crawling Insects, and Spiders			
1994 Included	0.222	0.221	1.01
1994 Excluded	0.232	0.100	2.31
Flying Insects	0.350	0.098	3.58
Crawling Insects	0.110	0.105	1.05
Crawling Insects & Spiders	0.153	0.102	1.50

Notes:
(a) Refer to Appendix D, Table D-2 for samples used to calculate the average concentration.
(b) BAF = Average Tissue Concentration/Average Soil Concentration
mg/kg = milligrams per kilogram
dw = dry weight

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TABLE 4-2

Summary of NOAEL, LOAEL, and Geometric Mean Target Concentrations in Tissue
OLIN McINTOSH OU-2

Receptor	MeHg				Hg (a)				DDTR			
	NOAEL Target (mg/kg)	LOAEL Target (mg/kg)	Geometric Mean Target (mg/kg)	Controlling Media	NOAEL Target (mg/kg)	LOAEL Target (mg/kg)	Geometric Mean Target (mg/kg)	Controlling Media	NOAEL Target (mg/kg)	LOAEL Target (mg/kg)	Geometric Mean Target (mg/kg)	Controlling Media
Carolina Wren	0.076	0.076	0.076	Invertebrates	0.16	0.16	0.16	Invertebrates	0.15	0.22	0.18	Invertebrates

Notes:
(a) Hg = MeHg/0.47; Assumes 47% of mercury is methylmercury.
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level
mg/kg = milligrams per kilogram

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TABLE 4-3

Calculation of Soil PRGs Based on Target Invertebrate Concentrations - Mercury
OLIN McINTOSH OU-2

Media	Allowed Invertebrate Tissue Concentration[a] for Methylmercury (mg/kg) (y)	Power Regression Equation	R^2	p-value	Power Target Soil Concentration for Mercury (mg/kg, dw) (x)	Linear Regression Equation	R^2	p-value	Linear Target Soil Concentration for Mercury (mg/kg, dw) (x)	Ratio Method	R^2	p-value	Ratio Method Target Soil Concentration for Mercury (mg/kg, dw) (x)
	NOAEL/LOAEL/ GEOMEAN[b]				NOAEL/LOAEL/ GEOMEAN[b]				NOAEL/LOAEL/ GEOMEAN[b]				NOAEL/LOAEL/ GEOMEAN[b]
Flying Insects, Crawling Insects, and Spiders													
1994 Included	0.076	$y = 0.0629x^{-0.292}$	0.043	0.5	0.52	$y = -0.0154x + 0.1182$	0.031	0.5	2.7	$y = 0.069x$	NA	NA	1.1
1994 Excluded	0.076	$y = 0.0607x^{-0.375}$	0.057	0.4	0.55	$y = -0.0178x + 0.1207$	0.022	0.6	2.5	$y = 0.081$	NA	NA	0.94
Spiders	0.076	$y = 0.0708x^{-0.165}$	0.49	0.5	0.65	$y = -0.0107x + 0.0831$	0.42	0.6	0.66	$y = 0.060x$	NA	NA	1.3
Flying Insects	0.076	$y = 0.1399x^{-0.078}$	0.021	0.8	2497	$y = -0.0018x + 0.1656$	0.00027	1.0	50	$y = 0.14x$	NA	NA	0.54
Crawling Insects	0.076	$y = 0.0257x^{-0.388}$	0.024	0.8	0.061	$y = -0.0259x + 0.0855$	0.077	0.7	0.37	$y = 0.039x$	NA	NA	1.9
Crawling Insects & Spiders	0.076	$y = 0.0378x^{-0.398}$	0.030	0.7	0.17	$y = -0.024x + 0.0889$	0.083	0.5	0.54	$y = 0.046x$	NA	NA	1.7

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Notes:
(a) The Carolina wren is the controlling ecological receptor for invertebrates (Table 4-2).
(b) As shown on Table 4-2, the NOAEL and LOAEL target invertebrate concentrations are the same, resulting in the same concentration for the geometric mean concentration.
NA = Not Applicable
PRG = Preliminary Remediation Goal
mg/kg = milligrams per kilogram
y = allowed invertebrate tissue concentration
x = target soil concentration
dw = dry weight
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level
GEOMEAN = Geometric mean of the NOAEL and LOAEL
■ Indicates the equation considered appropriate for PRG development due to power and linear analyses not achieving USEPA goals for R^2 values > 0.70 and significant p-values (<0.05).

TABLE 4-4a

Calculation of Soil PRGs Based on Target Invertebrate Concentrations - DDTR NOAEL
OLIN McINTOSH OU-2

Media	Allowed Invertebrate Tissue Concentration[a] for DDTR (mg/kg) (y)	Allowed Invertebrate Tissue Concentration[b] for DDTR (Normalized) (mg/kg) (y) (a)	Power Regression Equation	R^2	p-value	Power Target Soil Concentration[c] for DDTR (mg/kg, dw) (x)	Linear Regression Equation	R^2	p-value	Linear Target Soil Concentration[c] for DDTR (mg/kg, dw) (x)	Ratio Method	R^2	p-value	Ratio Method Target Soil Concentration[c] for DDTR (mg/kg, dw) (x)
Normalized Data	**NOAEL[d]**	**NOAEL[d]**				**NOAEL[d]**				**NOAEL[d]**				**NOAEL[d]**
Flying Insects, Crawling Insects, and Spiders														
1994 Included	0.15	4.17	$y = 3.1888x^{0.3221}$	0.11	0.3	0.17	y = -0.0499x + 6.4881	0.0056	0.8	3.5	y = 1.46x	NA	NA	0.21
1994 Excluded	0.15	4.17	$y = 3.0915x^{0.9136}$	0.33	0.08	0.10	y = 4.2354x - 0.2285	0.53	0.02	0.077	y = 4.09x	NA	NA	0.076
Spiders	0.15	4.17	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Flying Insects	0.15	3.95	$y = 5.9844x^{0.7376}$	0.89	0.06	0.023	y = 4.7889x + 0.474	0.83	0.09	0.030	y = 5.03x	NA	NA	0.032
Crawling Insects	0.15	4.29	$y = 1.3884x^{0.7811}$	0.19	0.6	0.40	y = 0.4519x + 2.6973	0.0054	0.9	0.33	y = 2.53x	NA	NA	0.16
Crawling Insects & Spiders	0.15	4.29	$y = 2.0679x^{0.933}$	0.24	0.3	0.19	y =1.9769x + 1.7104	0.12	0.5	0.12	y = 3.21x	NA	NA	0.11
Non-normalized Data														
Flying Insects, Crawling Insects, and Spiders														
1994 Included	0.15	NA	$y = 0.3314x^{0.3374}$	0.22	0.1	0.10	y = -0.0089x + 0.2245	0.00035	1.0	8.4	y = 1.01x	NA	NA	0.15
1994 Excluded	0.15	NA	$y = 0.6485x^{0.5297}$	0.35	0.07	0.063	y = 1.5884x + 0.0724	0.47	0.03	0.049	y = 2.31x	NA	NA	0.065
Spiders	0.15	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Flying Insects	0.15	NA	$y = 1.0305x^{0.4174}$	0.92	0.04	0.010	y = 2.233x + 0.1313	0.89	0.05	0.0085	y = 3.58x	NA	NA	0.042
Crawling Insects	0.15	NA	$y = 0.3673x^{0.6763}$	0.64	0.2	0.27	y = 1.2273x - 0.0183	0.55	0.3	0.11	y = 1.05x	NA	NA	0.14
Crawling Insects & Spiders	0.15	NA	$y = 0.5281x^{0.6426}$	0.47	0.1	0.14	y = 1.2027x + 0.0304	0.49	0.1	0.10	y = 1.50x	NA	NA	0.10

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Notes:
(a) The Carolina wren is the controlling ecological receptor for invertebrates (Table 4-2).
(b) Normalized target tissue concentrations calculated by dividing the target tissue concentration in Table 4-2 by the average fraction lipids for invertebrates samples.
Average fraction of lipids are as follows (Table D-2):
All Invertebrates (1994 Included/Excluded) - 0.036
Spiders - 0.036
Crawling Insects & Spiders - 0.035
Flying Insects - 0.038
Crawling Insects - 0.035
(c) Normalized soil concentrations denormalized by multiplying by the average FOC of associated soil samples; concentration presented is the non-normalized soil concentration.
Average fraction of organic carbon (FOC) are as follows (Table D-2):
All Invertebrates (1994 Included) - 0.0743
All Invertebrates (1994 Excluded) - 0.0743
Spiders - 0.0744
Crawling Insects & Spiders - 0.0856
Flying Insects - 0.0412
Crawling Insects - 0.0944
(d) NOAEL target invertebrate tissue concentration (Table 4-2).
NA = Not Applicable
PRG = Preliminary Remediation Goal
mg/kg = milligrams per kilogram
dw = dry weight
y = allowed invertebrate tissue concentration
x = target soil concentration
NOAEL = No Observed Adverse Effects Level
■ Indicates the equation considered appropriate for PRG development due to power and linear analyses not achieving USEPA goals for R2 values > 0.70 and significant p-values (<0.05) and the use of normalized data.

TABLE 4-4b

Calculation of Soil PRGs Based on Target Invertebrate Concentrations - DDTR LOAEL
OLIN McINTOSH OU-2

Media	Allowed Invertebrate Tissue Concentration[a] for DDTR (mg/kg) (y)	Allowed Invertebrate Tissue Concentration[b] for DDTR (Normalized) (mg/kg) (y) (a)	Power Regression Equation	R^2	p-value	Power Target Soil Concentration[c] for DDTR (mg/kg, dw) (x)	Linear Regression Equation	R^2	p-value	Linear Target Soil Concentration[c] for DDTR (mg/kg, dw) (x)	Ratio Method	R^2	p-value	Ratio Method Target Soil Concentration[c] for DDTR (mg/kg, dw) (x)
Normalized Data	**LOAEL[d]**	**LOAEL[d]**				**LOAEL[d]**				**LOAEL[d]**				**LOAEL[d]**
Flying Insects, Crawling Insects, and Spiders														
1994 Included	0.22	6.11	$y = 3.1888x^{0.3221}$	0.11	0.3	0.56	y = -0.0499x + 6.4881	0.0056	0.8	0.56	y = 1.46x	NA	NA	0.31
1994 Excluded	0.22	6.11	$y = 3.0915x^{0.9136}$	0.33	0.08	0.16	y = 4.2354x - 0.2285	0.53	0.02	0.11	y = 4.09x	NA	NA	0.11
Spiders	0.22	6.11	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Flying Insects	0.22	5.79	$y = 5.9844x^{0.7376}$	0.89	0.06	0.039	y = 4.7889x + 0.474	0.83	0.09	0.046	y = 5.03x	NA	NA	0.05
Crawling Insects	0.22	6.29	$y = 1.3884x^{0.7811}$	0.19	0.6	0.65	y = 0.4519x + 2.6973	0.0054	0.9	0.75	y = 2.53x	NA	NA	0.23
Crawling Insects & Spiders	0.22	6.29	$y = 2.0679x^{0.933}$	0.24	0.3	0.28	y =1.9769x + 1.7104	0.12	0.5	0.20	y = 3.21x	NA	NA	0.17
Non-normalized Data														
Flying Insects, Crawling Insects, and Spiders														
1994 Included	0.22	NA	$y = 0.3314x^{0.3374}$	0.22	0.1	0.30	y = -0.0089x + 0.2245	0.00035	1.0	0.51	y = 1.01x	NA	NA	0.22
1994 Excluded	0.22	NA	$y = 0.6485x^{0.5297}$	0.35	0.07	0.13	y = 1.5884x + 0.0724	0.47	0.03	0.093	y = 2.31x	NA	NA	0.095
Spiders	0.22	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Flying Insects	0.22	NA	$y = 1.0305x^{0.4174}$	0.92	0.04	0.025	y = 2.233x + 0.1313	0.89	0.05	0.040	y = 3.58x	NA	NA	0.061
Crawling Insects	0.22	NA	$y = 0.3673x^{0.6763}$	0.64	0.2	0.47	y = 1.2273x - 0.0183	0.55	0.3	0.16	y = 1.05x	NA	NA	0.21
Crawling Insects & Spiders	0.22	NA	$y = 0.5281x^{0.6426}$	0.47	0.1	0.26	y = 1.2027x + 0.0304	0.49	0.1	0.16	y = 1.50x	NA	NA	0.15

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Notes:
(a) The Carolina wren is the controlling ecological receptor for invertebrates (Table 4-2).
(b) Normalized target tissue concentrations calculated by dividing the target tissue concentration in Table 4-2 by the average fraction lipids for invertebrates samples.
Average fraction of lipids are as follows (Table D-2):
All Invertebrates (1994 Included/Excluded) - 0.036
Spiders - 0.036
Crawling Insects & Spiders - 0.035
Flying Insects - 0.038
Crawling Insects - 0.035
(c) Normalized soil concentrations denormalized by multiplying by the average FOC of associated soil samples; concentration presented is the non-normalized soil concentration.
Average fraction of organic carbon (FOC) are as follows (Table D-2):
All Invertebrates (1994 Included) - 0.0743
All Invertebrates (1994 Excluded) - 0.0743
Spiders - 0.0744
Crawling Insects & Spiders - 0.0856
Flying Insects - 0.0412
Crawling Insects - 0.0944
(d) LOAEL target invertebrate tissue concentration (Table 4-2).
NA = Not Applicable
PRG = Preliminary Remediation Goal
mg/kg = milligrams per kilogram
dw = dry weight
y = allowed invertebrate tissue concentration
x = target soil concentration
LOAEL = Lowest Observed Adverse Effects Level
■ Indicates the equation considered appropriate for PRG development due to power and linear analyses not achieving USEPA goals for R^2 values > 0.70 and significant p-values (<0.05) and the use of normalized data.

TABLE 4-4c

Calculation of Soil PRGs Based on Target Invertebrate Concentrations - DDTR Geometric Mean
OLIN McINTOSH OU-2

Media	Allowed Invertebrate Tissue Concentration[a] for DDTR (mg/kg) (y)	Allowed Invertebrate Tissue Concentration[b] for DDTR (Normalized) (mg/kg) (y) (a)	Power Regression Equation	R^2	p-value	Power Target Soil Concentration[c] for DDTR (mg/kg, dw) (x)	Linear Regression Equation	R^2	p-value	Linear Target Soil Concentration[c] for DDTR (mg/kg, dw) (x)	Ratio Method	R^2	p-value	Ratio Method Target Soil Concentration[c] for DDTR (mg/kg, dw) (x)
Normalized Data	**GEOMEAN[d]**	**GEOMEAN[d]**				**GEOMEAN[d]**				**GEOMEAN[d]**				**GEOMEAN[d]**
Flying Insects, Crawling Insects, and Spiders														
1994 Included	0.18	5.00	$y = 3.1888x^{0.3221}$	0.11	0.3	0.30	y = -0.0499x + 6.4881	0.0056	0.8	2.2	y = 1.46x	NA	NA	0.25
1994 Excluded	0.18	5.00	$y = 3.0915x^{0.9136}$	0.33	0.08	0.13	y = 4.2354x - 0.2285	0.53	0.02	0.092	y = 4.09x	NA	NA	0.091
Spiders	0.18	5.00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Flying Insects	0.18	4.74	$y = 5.9844x^{0.7376}$	0.89	0.06	0.030	y = 4.7889x + 0.474	0.83	0.09	0.037	y = 5.03x	NA	NA	0.039
Crawling Insects	0.18	5.14	$y = 1.3884x^{0.7811}$	0.19	0.6	0.50	y = 0.4519x + 2.6973	0.0054	0.9	0.51	y = 2.53x	NA	NA	0.19
Crawling Insects & Spiders	0.18	5.14	$y = 2.0679x^{0.933}$	0.24	0.3	0.23	y =1.9769x + 1.7104	0.12	0.5	0.15	y = 3.21x	NA	NA	0.14
Non-normalized Data														
Flying Insects, Crawling Insects, and Spiders														
1994 Included	0.18	NA	$y = 0.3314x^{0.3374}$	0.22	0.1	0.16	y = -0.0089x + 0.2245	0.00035	1.0	5.0	y = 1.01x	NA	NA	0.18
1994 Excluded	0.18	NA	$y = 0.6485x^{0.5297}$	0.35	0.07	0.089	y = 1.5884x + 0.0724	0.47	0.03	0.068	y = 2.31x	NA	NA	0.078
Spiders	0.18	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Flying Insects	0.18	NA	$y = 1.0305x^{0.4174}$	0.92	0.04	0.015	y = 2.233x + 0.1313	0.89	0.05	0.022	y = 3.58x	NA	NA	0.050
Crawling Insects	0.18	NA	$y = 0.3673x^{0.6763}$	0.64	0.2	0.35	y = 1.2273x - 0.0183	0.55	0.3	0.13	y = 1.05x	NA	NA	0.17
Crawling Insects & Spiders	0.18	NA	$y = 0.5281x^{0.6426}$	0.47	0.1	0.19	y = 1.2027x + 0.0304	0.49	0.1	0.13	y = 1.50x	NA	NA	0.12

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Notes:
(a) The Carolina wren is the controlling ecological receptor for invertebrates (Table 4-2).
(b) Normalized target tissue concentrations calculated by dividing the target tissue concentration in Table 4-2 by the average fraction lipids for invertebrates samples.
Average fraction of lipids are as follows (Table D-2):
All Invertebrates (1994 Included/Excluded) - 0.036
Spiders - 0.036
Crawling Insects & Spiders - 0.035
Flying Insects - 0.038
Crawling Insects - 0.035
(c) Normalized soil concentrations denormalized by multiplying by the average FOC of associated soil samples; concentration presented is the non-normalized soil concentration.
Average fraction of organic carbon (FOC) are as follows (Table D-2):
All Invertebrates (1994 Included) - 0.0743
All Invertebrates (1994 Excluded) - 0.0743
Spiders - 0.0744
Crawling Insects & Spiders - 0.0856
Flying Insects - 0.0412
Crawling Insects - 0.0944
(d) Geometric mean of the NOAEL and LOAEL target invertebrate tissue concentrations (Table 4-2).
NA = Not Applicable
PRG = Preliminary Remediation Goal
mg/kg = milligrams per kilogram
dw = dry weight
y = allowed invertebrate tissue concentration
x = target soil concentration
GEOMEAN = Geometric mean of the NOAEL and LOAEL
■ Indicates the equation considered appropriate for PRG development due to power and linear analyses not achieving USEPA goals for R^2 values > 0.70 and significant p-values (<0.05) and the use of normalized data.

TABLE 4-5

Summary of Mercury PRGs for Floodplain Soil - Based on Risk from Invertebrates
OLIN McINTOSH OU-2

	Range of Target Soil Concentrations Protective of Carolina Wren (mg/kg, dw)									
Media	**Power Analysis**	**R^2**	**p-value**	**Linear Analysis**	**R^2**	**p-value**	**Ratio Method**	**R^2**	**p-value**	**Range of Soil PRGs (mg/kg)**
Flying Insects, Crawling Insects, and Spiders	**NOAEL/LOAEL/ GEOMEAN[(b)]**			**NOAEL/LOAEL/ GEOMEAN[(b)]**			**NOAEL/LOAEL/ GEOMEAN[(b)]**			
1994 Included	0.52	0.043	0.5	2.7	0.031	0.5	1.1	NA	NA	
1994 Excluded	0.55	0.057	0.4	2.5	0.022	0.6	0.94	NA	NA	
OVERALL RANGE	NA [(a)]			NA [(a)]			**0.94 - 1.1**			**0.94 - 1.1**
Spiders	0.65	0.49	0.5	0.66	0.42	0.6	1.3	NA	NA	
OVERALL RANGE	NA [(a)]			NA [(a)]			**1.3**			**1.3**
Flying Insects	2497	0.021	0.8	50	0.00027	1.0	0.54	NA	NA	
OVERALL RANGE	NA [(a)]			NA [(a)]			**0.54**			**0.54**
Crawling Insects	0.061	0.024	0.8	0.37	0.077	0.7	1.9	NA	NA	
OVERALL RANGE	NA [(a)]			NA [(a)]			**1.9**			**1.9**
Crawling Insects & Spiders	0.17	0.030	0.7	0.54	0.083	0.5	1.7	NA	NA	
OVERALL RANGE	NA [(a)]			NA [(a)]			**1.7**			**1.7**
							OVERALL RANGE OF MERCURY FLOODPLAIN SOIL PRG (mg/kg) [(a)] (Across all Exposure Scenarios)			**0.54 - 1.9**

Notes:

(a) The low R^2 values (< 0.70) and unacceptable p-values (>0.05) indicate a higher level of uncertainty with the soil values calculated. Target soil concentrations derived only from equations with R^2 > 0.70 and significant p-values and the ratio method are the focus of PRG development. Power and linear analyses with R^2 values <0.70 and unacceptable p-values shown for informational purposes only.

(b) As shown on Table 4-2, the NOAEL and LOAEL target invertebrate concentrations are the same, resulting in the same concentration for the geometric mean concentration.

NA = Not Applicable
PRG = Preliminary Remediation Goal
mg/kg = milligrams per kilogram
dw = dry weight
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level
GEOMEAN = Geometric mean of the NOAEL and LOAEL

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CHECKED BY/DATE: EFC 4/15/12

■ Indicates the equation considered appropriate for PRG development due to power and linear analyses not achieving USEPA goals for R^2 values > 0.70 and significant p-values (<0.05).

TABLE 4-6

Summary of DDTR PRGs for Floodplain Soil - Based on Risk from Invertebrates
OLIN McINTOSH OU-2

Media	Range of Target Soil Concentrations Protective of Carolina Wren (mg/kg, dw)															
	Power Analysis			R^2	p-value	Linear Analysis			R^2	p-value	Ratio Method			R^2	p-value	Overall Range of Soil PRGs (mg/kg)
	NOAEL	LOAEL	GEOMEAN			NOAEL	LOAEL	GEOMEAN			NOAEL	LOAEL	GEOMEAN			
Normalized Data																
Flying Insects, Crawling Insects, and Spiders																
1994 Included	0.17	0.56	0.30	0.11	0.3	3.5	0.56	2.2	0.0056	0.8	0.21	0.31	0.25	NA	NA	
1994 Excluded	0.10	0.16	0.13	0.33	0.08	0.077	0.11	0.092	0.53	0.02	0.076	0.11	0.091	NA	NA	
Spiders	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	
Flying Insects	0.023	0.039	0.030	0.89	0.06	0.030	0.046	0.037	0.83	0.09	0.032	0.047	0.039	NA	NA	
Crawling Insects	0.40	0.65	0.50	0.19	0.6	0.33	0.75	0.51	0.0054	0.9	0.16	0.23	0.19	NA	NA	
Crawling Insects & Spiders	0.19	0.28	0.23	0.24	0.3	0.12	0.20	0.15	0.12	0.5	0.11	0.17	0.14	NA	NA	
OVERALL RANGE	NA [(a)]	NA [(a)]	NA [(a)]			NA [(a)]	NA [(a)]	NA [(a)]			**0.032 - 0.21**	**0.047 - 0.31**	**0.039 - 0.25**			**0.032 - 0.31**
Non-normalized Data																
Flying Insects, Crawling Insects, and Spiders																
1994 Included	0.10	0.30	0.16	0.22	0.1	8.4	0.51	5.0	0.00035	1.0	0.15	0.22	0.18	NA	NA	
1994 Excluded	0.063	0.13	0.089	0.35	0.07	0.049	0.093	0.068	0.47	0.03	0.065	0.095	0.078	NA	NA	
Spiders	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	
Flying Insects	0.010	0.025	0.015	0.92	0.04	0.0085	0.040	0.022	0.89	0.05	0.042	0.061	0.050	NA	NA	
Crawling Insects	0.27	0.47	0.35	0.64	0.2	0.11	0.16	0.13	0.55	0.3	0.14	0.21	0.17	NA	NA	
Crawling Insects & Spiders	0.14	0.26	0.19	0.47	0.1	0.10	0.16	0.13	0.49	0.1	0.10	0.15	0.12	NA	NA	
OVERALL RANGE	**0.010** [(a)]	**0.025** [(a)]	**0.015** [(a)]			NA [(a)]	NA [(a)]	NA [(a)]			**0.042 - 0.15**	**0.061 - 0.22**	**0.050 - 0.18**			**0.010 - 0.22**
													OVERALL RANGE OF DDTR FLOODPLAIN SOIL PRG (mg/kg) [(a)] (Across All Types of Analysis)			**0.010 - 0.31**

Notes:

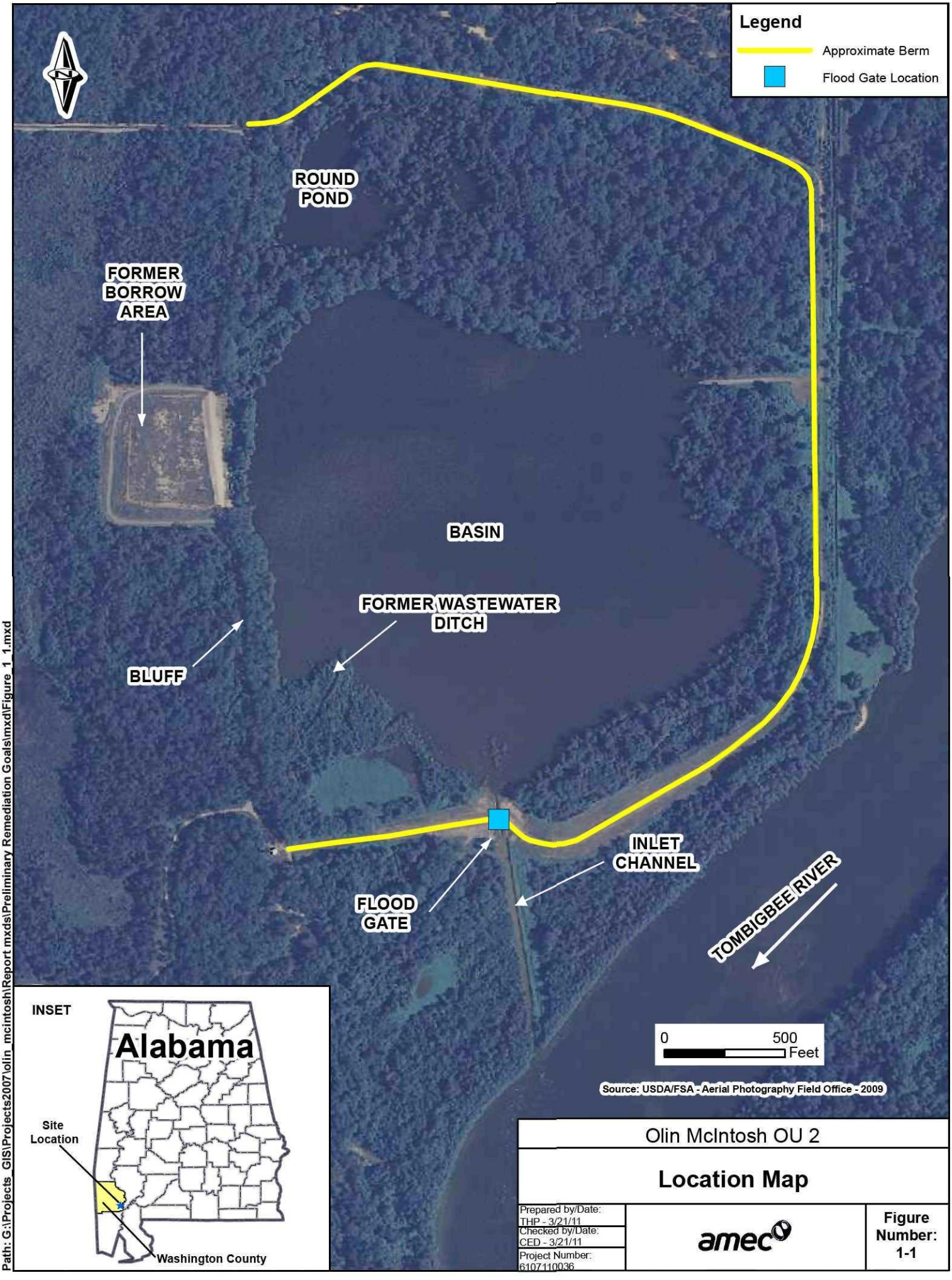
(a) The low R^2 values (< 0.70) and unacceptable p-values (>0.05) indicate a higher level of uncertainty with the soil values calculated. Target soil concentrations derived only from equatio
with R^2 > 0.70 and significant p-values and the ratio method are the focus of PRG development. Power and linear analyses with I^2 values <0.70 and unacceptable p-values shown for informational purposes only.

NA = Not Applicable
PRG = Preliminary Remediation Goal
NOAEL = No Observed Adverse Effects Level
LOAEL = Lowest Observed Adverse Effects Level
GEOMEAN = Geometric mean of the NOAEL and LOAEL
mg/kg = milligrams per kilogram
dw = dry weight

■ Indicates the equation considered appropriate for PRG development due to power and linear analyses not achieving USEPA goals for R^2 values > 0.70 and significant p-values (<0.05) and the use of normalized data.

PREPARED BY/DATE: NSR 4/15/12
CHECKED BY/DATE: EFC 4/15/12

FIGURES



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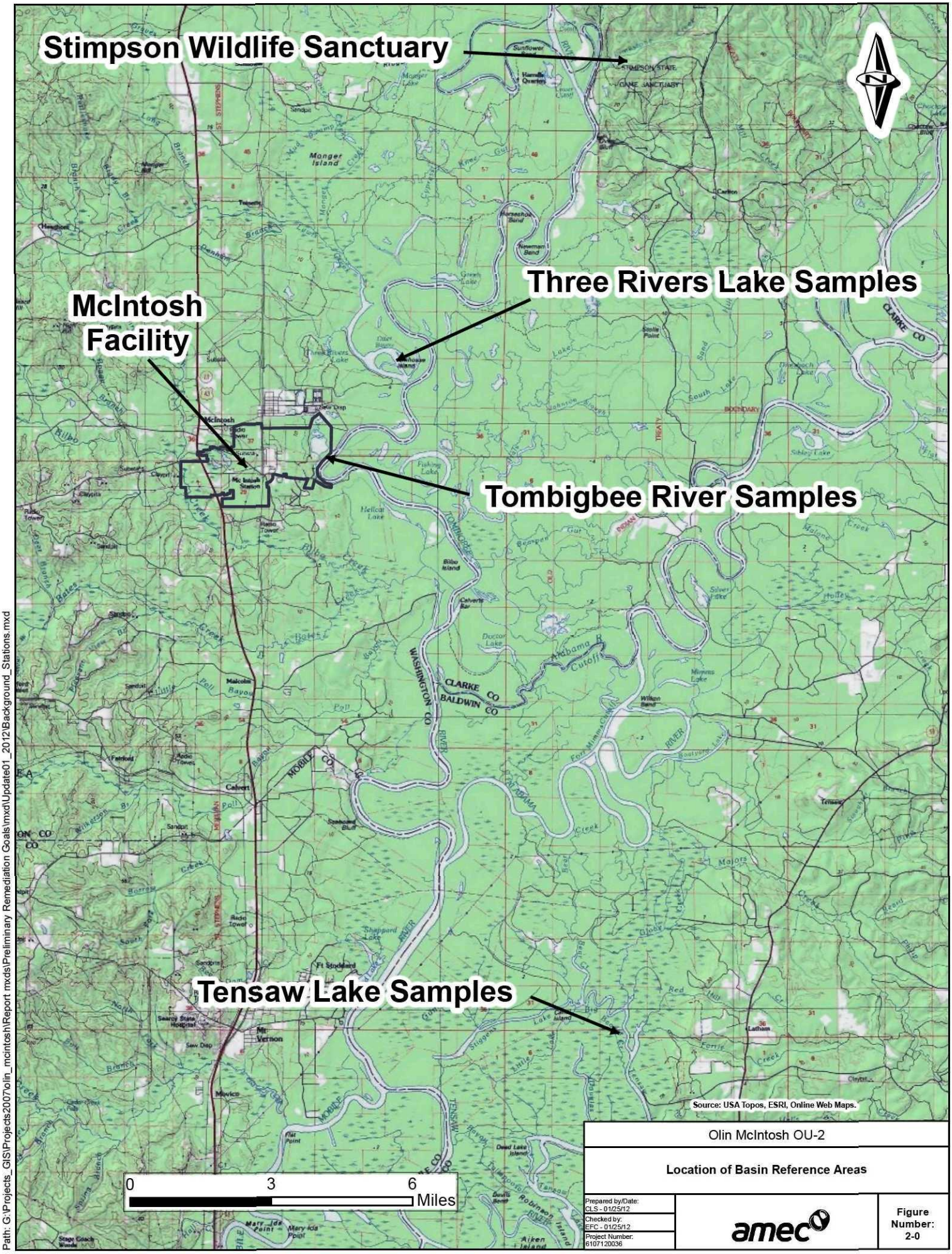
Olin McIntosh OU 2

Location Map

Prepared by/Date: THP - 3/21/11 Checked by/Date: CED - 3/21/11 Project Number: 6107110036	amec	Figure Number: 1-1



Olin McIntosh OU-2

Location of Basin Reference Areas

Prepared by/Date: CLS - 01/25/12 Checked by: EFC - 01/25/12 Project Number: 6107120036	amec	Figure Number: 2-0

Path: G:\Projects_GIS\Projects2007\olin_mcintosh\Report mxds\Preliminary Remediation Goals\mxd\Update01_2012\Background_Stations.mxd

OLE0204-0694
OLE0201-0694
G05-94
RP Basin
ROUND POND
OLE0206-0694
D11-91
OLE0105-0694
B10-91
C10-91
D10-91
E10-91
F10-91
H10-91
I10-91
H9-91
B9-91
C9-91
D9-91
E9-91
F9-91
G09-91
I9-91
J9-91
NW Basin
NE Basin
G03-94
B8-91
C8-91
D8-91
E8-91
F8-91
G08-91
H8-91
I8-91
OLE0107-0694
OLE0108-0694
OLE0109-0694
I7-91SC
I7-91SED
J7-91
A7
B7-91
C7-91
D7-91
E7-91
F7-91
G07-91
H7-91
OLE0103-0694
BASIN
OLE0102-0694
B6-91
C6-91
D6-91
E6-91
F6-91
G06-91
H6-91
I6-91
J6-91
H5-91
B5-91
C5-91
D5-91
E5-91
F5-91
G05-91
I5-91
J5-91
K5-91
G01-94
B4-91
C4-91
D4-91
E4-91
F4-91
G04-91
H4-91
I4-91
J4-91
K4-91
K4-91
SW Basin
SE Basin
D3-91
E3-91
F3-91
G03-91
H3-91
I3-91
J3-91
E2
E2-91SC
F2-91
G02-91
H2-91
F1-91
G01-91
INLET CHANNEL
TOMBIGBEE RIVER

Source: USDA/FSA - Aerial Photography Field Office - 2009

Legend

- 1991-1992 Sediment Sample Location
- 1994 Sediment Sample Location
- 1994 Predatory Fish Sample Location
- Predatory Fish Grid

0 200 400 600 800 Feet

Note: The location of the 1991 fish samples are not included due to unknown locations. 1991 fish data included with data pairing on Table A-1.

Olin McIntosh OU-2

1991 & 1994 Predatory Fish and Sediment Data Pairings

Prepared by/Date: SLW - 03/21/11	amec	Figure Number: 2-1
Checked by: EFC - 03/21/11		
Project Number: 6107110036		

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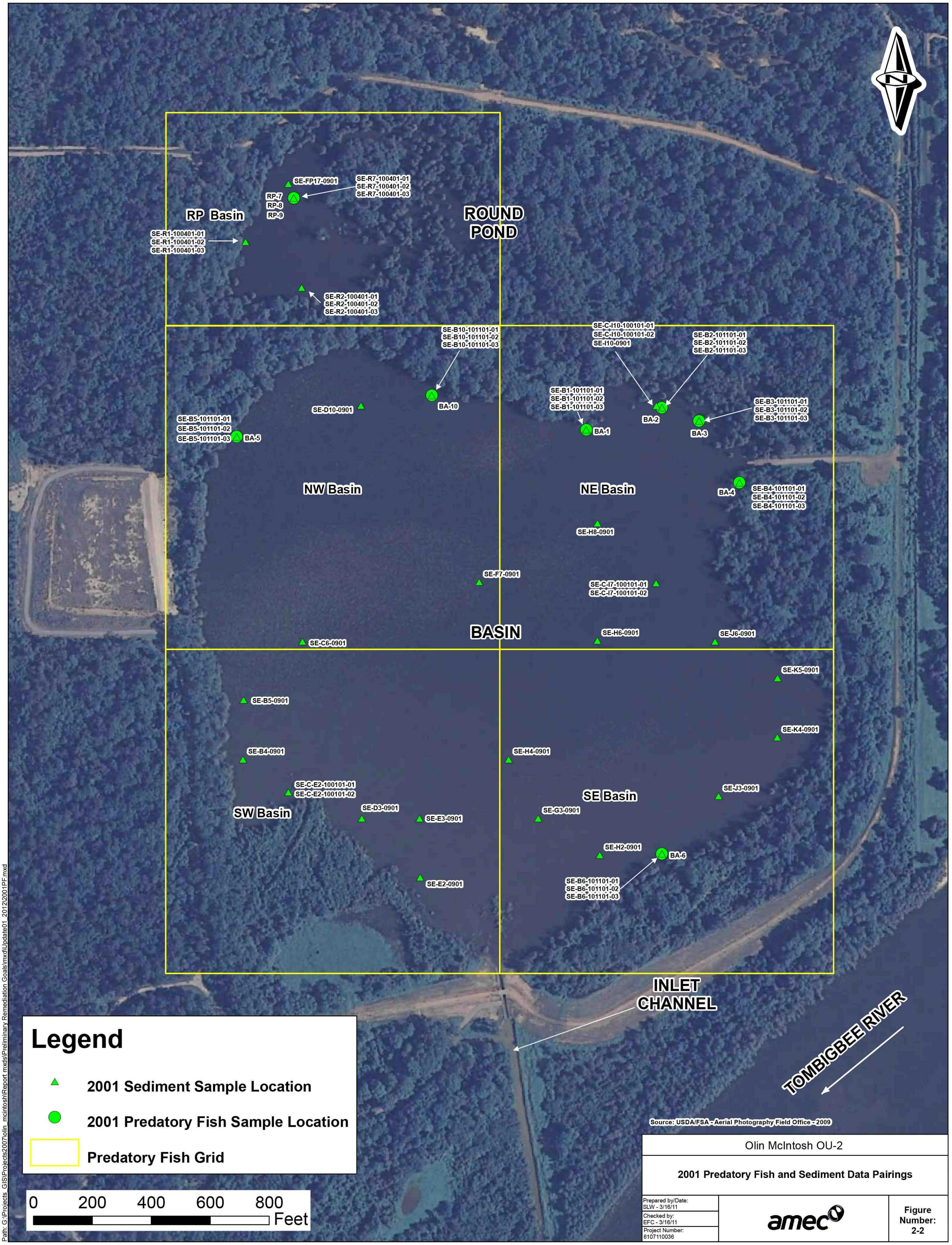

Legend

- 2001 Sediment Sample Location
- 2001 Predatory Fish Sample Location
- Predatory Fish Grid

0 200 400 600 800 Feet

Olin McIntosh OU-2

2001 Predatory Fish and Sediment Data Pairings

Prepared by/Date: SLW - 3/16/11	amec	Figure Number: 2-2
Checked by: EFC - 3/16/11		
Project Number: 6107110036		

Path: G:\Projects_GIS\Projects2007\olin_mcintosh\Report mxds\Preliminary Remediation Goals\mxd\Update01_2012\2001PF.mxd

RP Basin

ROUND POND

NW Basin

NE Basin

BASIN

SW Basin

SE Basin

INLET CHANNEL

TOMBIGBEE RIVER

OU2B-SED-501D-08 (5 pt. composite)

OU2B-SED-502D-08 (5 pt. composite)

OU2B-SED-401C-08

OU2B-SED-402C-08

OU2B-SED-403C-08

OU2B-SED-404C-08

OU2B-SED-004C-08

OU2B-SED-101C-08

OU2B-SED-102C-08

OU2B-SED-103D-08 (5 pt. composite)

OU2B-SED-106C-08

OU2B-SED-105C-08

OU2B-SED-104D-08 (5 pt. composite)

OU2B-SED-203D-08 (5 pt. composite)

OU2B-SED-201C-08

OU2B-SED-202D-08 (5 pt. composite)

OU2B-SED-204C-08

OU2B-SED-205C-08

OU2B-SED-301C-08

OU2B-SED-302C-08

OU2B-SED-303D-08 (5 pt. composite)

OU2B-SED-304C-08

MCI-0021-08WB-NE
MCI-0022-08WB-NE
MCI-0023-08WB-NE
MCI-0024-08WB-NE
MCI-0043-08WB-NE
MCI-0054-08WB-NE
MCI-0055-08WB-NE
MCI-0056-08WB-NE
MCI-0057-08WB-NE
MCI-0058-08WB-NE

MCI-0025-08WB-NW
MCI-0026-08WB-NW
MCI-0027-08WB-NW
MCI-0028-08WB-NW
MCI-0029-08WB-NW
MCI-0044-08WB-NW
MCI-0045-08WB-NW
MCI-0046-08WB-NW
MCI-0047-08WB-NW
MCI-0048-08WB-NW

MCI-0030-08WB-SW
MCI-0031-08WB-SW
MCI-0032-08WB-SW
MCI-0033-08WB-SW
MCI-0034-08WB-SW
MCI-0049-08WB-SW
MCI-0050-08WB-SW
MCI-0051-08WB-SW
MCI-0052-08WB-SW
MCI-0053-08WB-SW

MCI-0035-08WB-SE
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MCI-0040-08WB-SE
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MCI-0059-08WB-SE
MCI-0060-08WB-SE

Legend

- 2008 Sediment Sample Location
- 2008 Predatory Fish Sample Location
- Predatory Fish Grid

0 200 400 600 800 Feet

Source: USDA/FSA - Aerial Photography Field Office - 2009

Olin McIntosh OU-2

2008 Predatory Fish and Sediment Data Pairings

Prepared by/Date: SLW - 3/16/11	amec	Figure Number: 2-3
Checked by: EFC - 3/16/11		
Project Number: 6107110036		

Path: G:\Projects_GIS\Projects2007\olin_mcintosh\Report mxds\Preliminary Remediation Goals\mxd\Update01_2012\2008PF.mxd

FP12-92
FP13-92
G05-94
FP17-92
FP18-92
FP19-92
ROUND POND
OGS0308-0694
OGS0309-0694
FP20-92
FP21-92
FP22-92
D11-91
B10-91
C10-91
D10-91
E10-91
F10-91
H10-91
I10-91
B9-91
C9-91
D9-91
E9-91
F9-91
G09-91
H9-91
I9-91
J9-91
G03-94
B8-91
C8-91
D8-91
E8-91
F8-91
G08-91
H8-91
I8-91
OGS0101-0694
OGS0102-0694
OGS0103-0694
A7
B7-91
C7-91
D7-91
E7-91
F7-91
G07-91
H7-91
I7-91SC
I7-91SED
J7-91
BASIN
B6-91
C6-91
D6-91
E6-91
F6-91
G06-91
H6-91
I6-91
J6-91
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C5-91
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F5-91
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J5-91
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G04-91
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I4-91
J4-91
K4-91
K4-91
D3-91
E3-91
F3-91
G03-91
H3-91
I3-91
J3-91
E2
E2-91SC
F2-91
G02-91
H2-91
F1-91
G01-91
INLET CHANNEL
TOMBIGBEE RIVER

Source: USDA/FSA - Aerial Photography Field Office - 2009

Legend

- 1991-1992 Sediment Sample Location
- 1994 Sediment Sample Location
- 1994 Forage Fish Sample Location (Mosquito Fish)
- 400 Foot Forage Area

0 200 400 600 800 Feet

Olin McIntosh OU-2

1991 & 1994 Forage Fish and Sediment Data Pairings

Prepared by/Date: SLW - 01/31/12	amec	Figure Number: 2-4
Checked by: EFC - 01/31/12		
Project Number: 6107110036		

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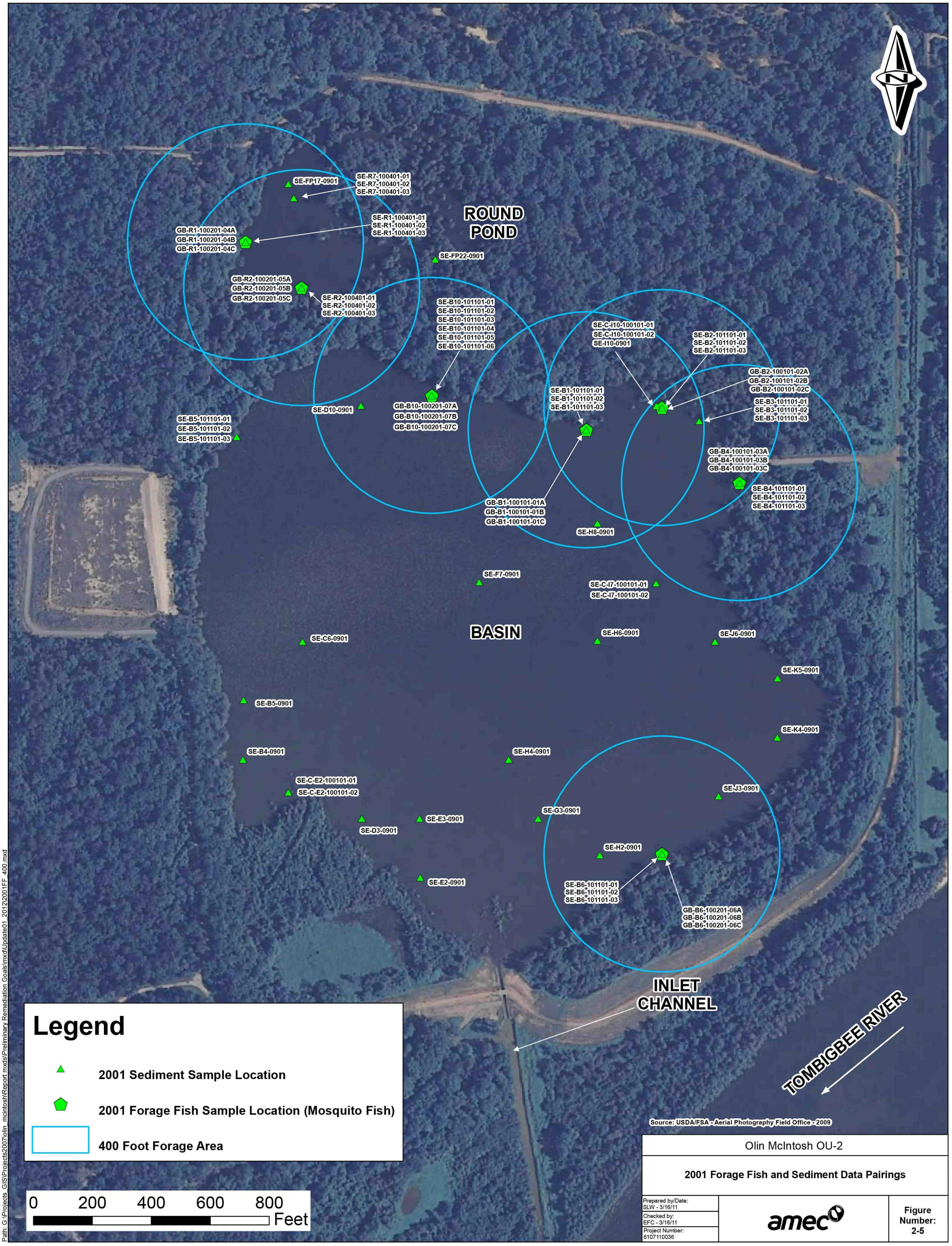
ROUND POND
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SE-R7-100401-01
SE-R7-100401-02
SE-R7-100401-03
SE-R1-100401-01
SE-R1-100401-02
SE-R1-100401-03
GB-R1-100201-04A
GB-R1-100201-04B
GB-R1-100201-04C
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SE-B10-101101-02
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SE-B10-101101-06
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GB-B1-100101-01C
SE-H8-0901
SE-F7-0901
SE-C-I7-100101-01
SE-C-I7-100101-02
BASIN
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SE-H6-0901
SE-J6-0901
SE-K5-0901
SE-B5-0901
SE-K4-0901
SE-B4-0901
SE-H4-0901
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SE-B6-101101-03
GB-B6-100201-06A
GB-B6-100201-06B
GB-B6-100201-06C
INLET CHANNEL
TOMBIGBEE RIVER
Source: USDA/FSA - Aerial Photography Field Office - 2009
Legend
2001 Sediment Sample Location
2001 Forage Fish Sample Location (Mosquito Fish)
400 Foot Forage Area
0 200 400 600 800
Feet
Path: G:\Projects_GIS\Projects2007\olin_mcintosh\Report mxds\Preliminary Remediation Goals\mxd\Update01_20122001FF_400.mxd
Olin McIntosh OU-2
2001 Forage Fish and Sediment Data Pairings
Prepared by/Date: SLW - 3/16/11
Checked by: EFC - 3/16/11
Project Number: 6107110036
amec
Figure Number: 2-5

ROUND POND

BASIN

INLET CHANNEL

TOMBIGBEE RIVER

OU2B-SED-501DC-08
OU2B-SED-401C-08
OU2B-SED-402C-08
OU2B-SED-101C-08
OU2B-SED-102C-08
OU2B-SED-103DC-08
OU2B-SED-201C-08
OU2B-SED-202DC-08
OU2B-SED-203DC-08
OU2B-SED-301C-08
OU2B-SED-302C-08
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OU2B-SED-304C-08
OU2B-SED-502DC-08
OU2B-SED-403C-08
OU2B-SED-404C-08
OU2B-SED-004C-08
OU2B-SED-104DC-08
OU2B-SED-105C-08
OU2B-SED-106C-08
OU2B-SED-204C-08
OU2B-SED-205C-08

MCI-0066-08WB-NW
MCI-0067-08WB-NW
MCI-0068-08WB-NW
MCI-0069-08WB-NW
MCI-0070-08WB-NW
MCI-0085-08WB-NW

MCI-0076-08WB-SW
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MCI-0078-08WB-SW
MCI-0079-08WB-SW
MCI-0080-08WB-SW
MCI-0084-08WB-SW

MCI-0061-08WB-NE
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MCI-0072-08WB-SE
MCI-0073-08WB-SE
MCI-0074-08WB-SE
MCI-0075-08WB-SE
MCI-0083-08WB-SE

Legend

- 2008 Forage Fish Sample Location (Silverside)
- 2008 Forage Fish Sample Location (Bluegill)
- 2008 Sediment Sample Location
- 400 Foot Forage Area

0 200 400 600 800 Feet

Source: USDA/FSA - Aerial Photography Field Office - 2009

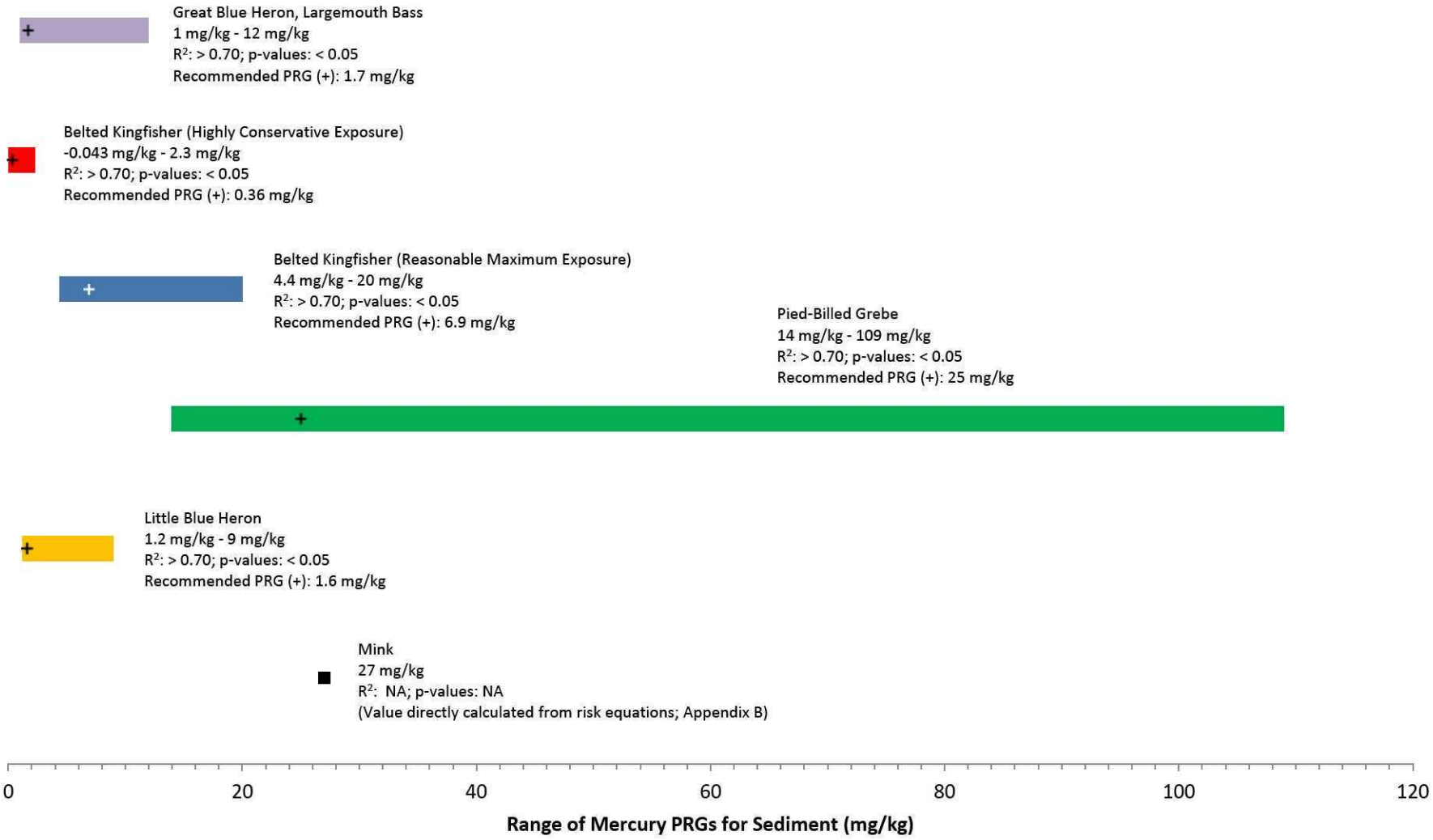
Olin McIntosh OU-2

2008 Forage Fish and Sediment Data Pairings

Prepared by/Date: SLW - 3/16/11	amec	Figure Number: 2-6
Checked by: EFC - 3/16/11		
Project Number: 6107110036		

Path: G:\Projects_GIS\Projects2007\olin_mcintosh\Report mxds\Preliminary Remediation Goals\mxd\Update01_2012\2008FF_400.mxd

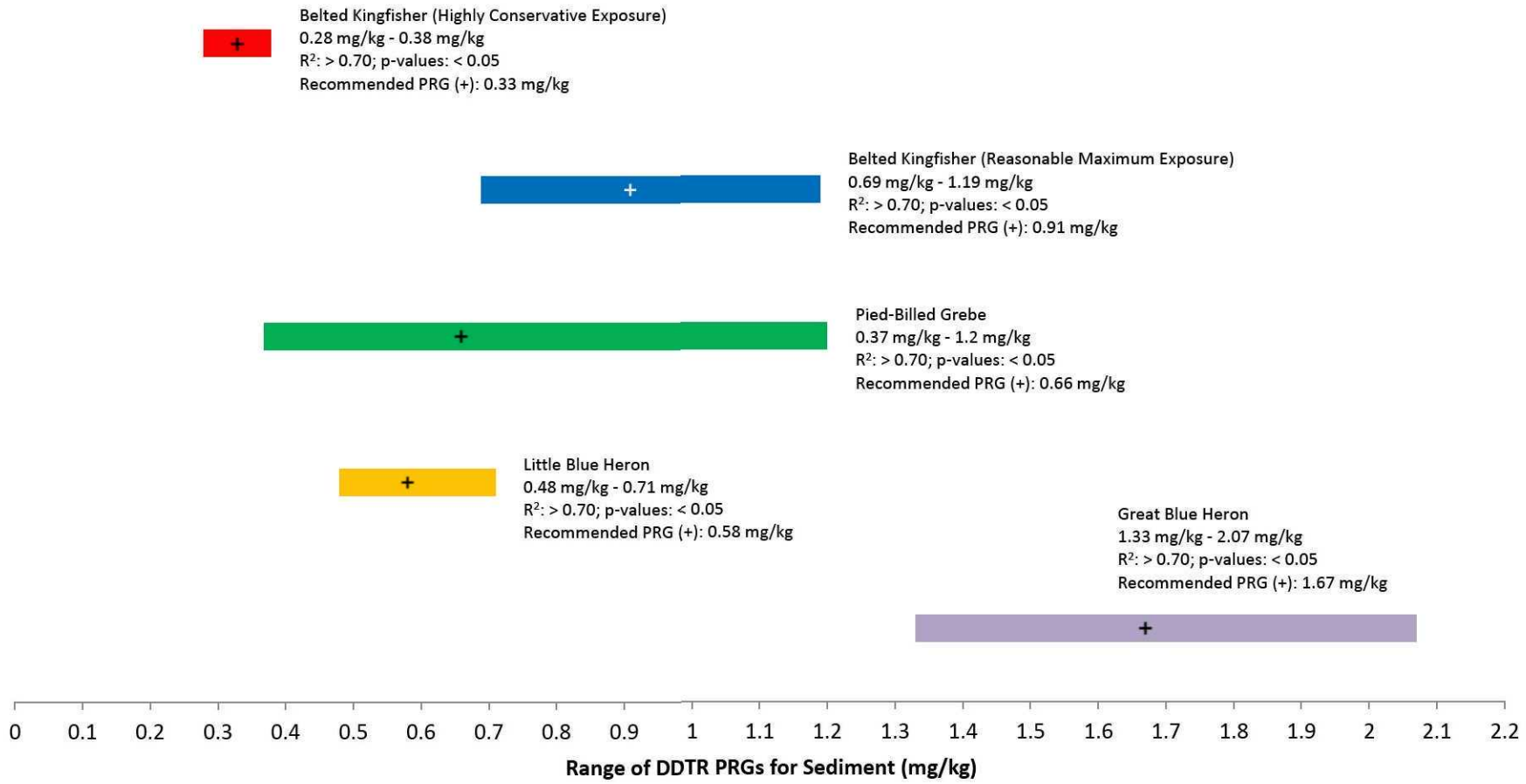
Figure 2-7
Mercury Target Sediment Concentrations Protective of Receptor Based on Risk from Forage and Predatory Fish



+ Indicates the PRG for the receptor using the combined dataset (Table 2-8 and Table 2-9).

PREPARED BY/DATE: MKB 3/28/12
CHECKED BY/DATE: EFC 3/28/12

Figure 2-8
DDTR Target Sediment Concentrations Protective of Receptor Based on Risk from Forage Fish



+ Indicates the geometric mean PRG for the receptor (Table 2-10).

PREPARED BY/DATE: MKB 3/28/12
CHECKED BY/DATE: EFC 3/28/12

ROUND POND

BASIN

INLET CHANNEL

TOMBIGBEE RIVER

OU2B-FPSS1-10
OIN0509
OIN0508
OIN0507
OU2B-FPSS6-10
OU2B-IN S1-10
OU2B-IN SNE-10
OU2B-FPSS8-10
OU2B-FPSB1-10-0-1
OU2B-FPSS4-10
OU2B-IN S2-10
OU2B-IN SNE-10
OSGO901
OSGO902
OSGO903
OSGO903FD
OU2B-FPSB3-10-0-1
OU2B-IN S3-10
OU2B-IN SNE-10
OU2B-FPSS3-10
OU2B-FPSS7-10
OU2B-FPSS2-10
OU2B-FPSS5-10
OU2B-FPSB2-10-0-1
OIN0202
OIN0705
OU2B-FPSS9-10
OU2B-FPSS10-10
ODGO801
ODGO802
ODGO803
OU2B-FPSB4-10-0-1
OIN0404
OSGO701
OSGO701FD
OSGO702
OSGO703
OIN0303
OU2B-FPSS11-10
OU2B-IN S4-10
OU2B-IN SSE-10
OU2B-FPSS15-10
OIN0101
OU2B-FPSB5-10-0-1
OU2B-IN S5-10
OU2B-IN SSE-10
OIN0806
OU2B-FPSS12-10
OU2B-FPSS14-10
OU2B-IN S6-10
OU2B-FPSS13-10
OU2B-FPSB6-10-0-1

Source: USDA/FSA - Aerial Photography Field Office - 2009

Legend

- 1994 Insect Sample Location
- 2010 Insect Sample Location
- 1994 Floodplain Soil Sample Location
- 2010 Floodplain Soil Sample Location
- 2010 Composite Insect Samples
- 1994, 400 Foot Forage Area (Included in Regression Line for Figure D-5A only)
- 2010, 400 Foot Forage Area

0 200 400 600 800 Feet

Path: G:\Projects_GIS\Projects2007\olin_mcintosh\Report mxds\Preliminary Remediation Goals\mxdUpdate01_2012\Combo_Soil_Insect.mxd

Olin McIntosh OU-2

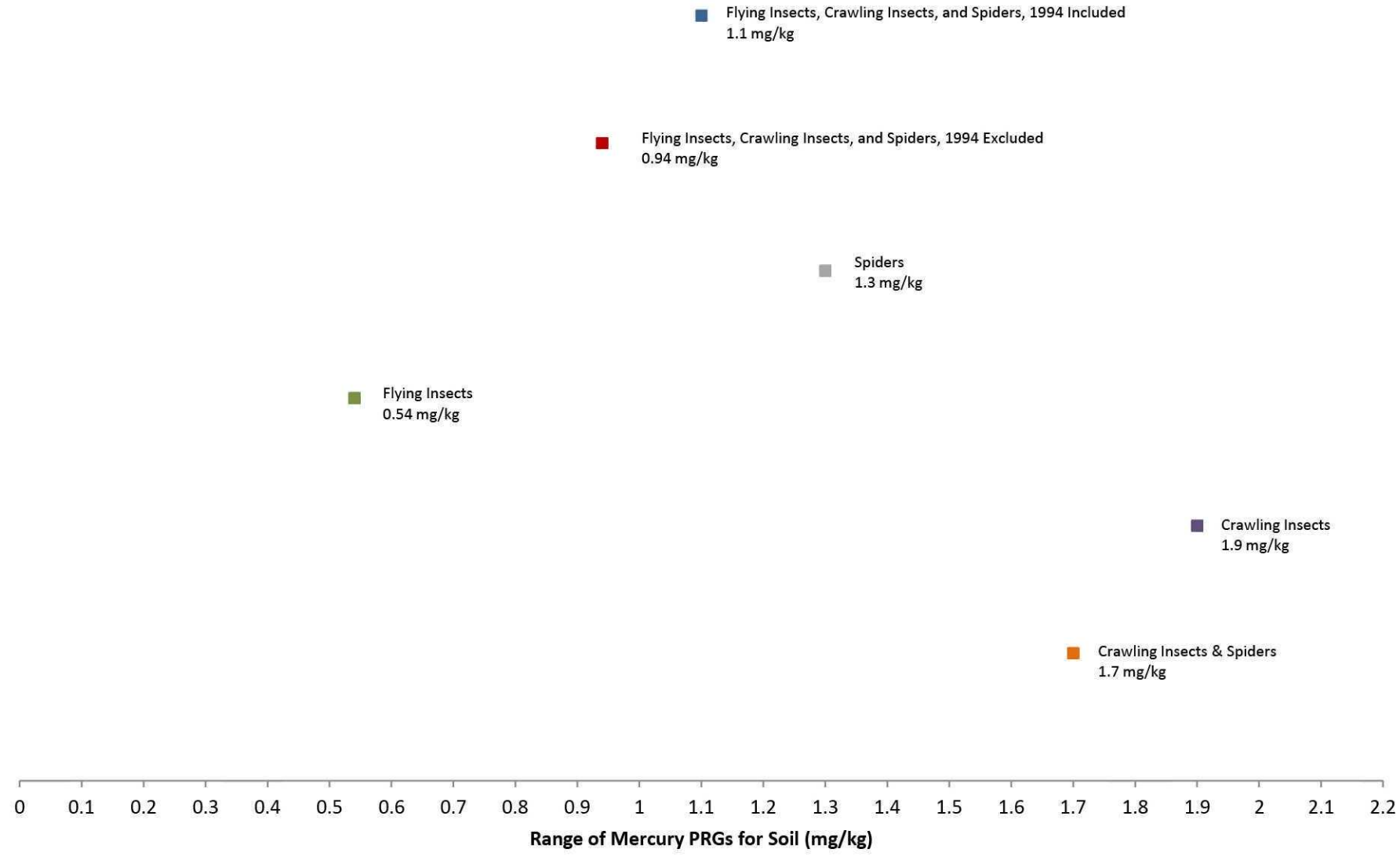
1994 and 2010 Invertebrate and Floodplain Soil Data Pairings

Prepared by/Date:	SLW - 01/23/12
Checked by:	EFC - 01/23/12
Project Number:	6107110036

amec

Figure Number: 4-1

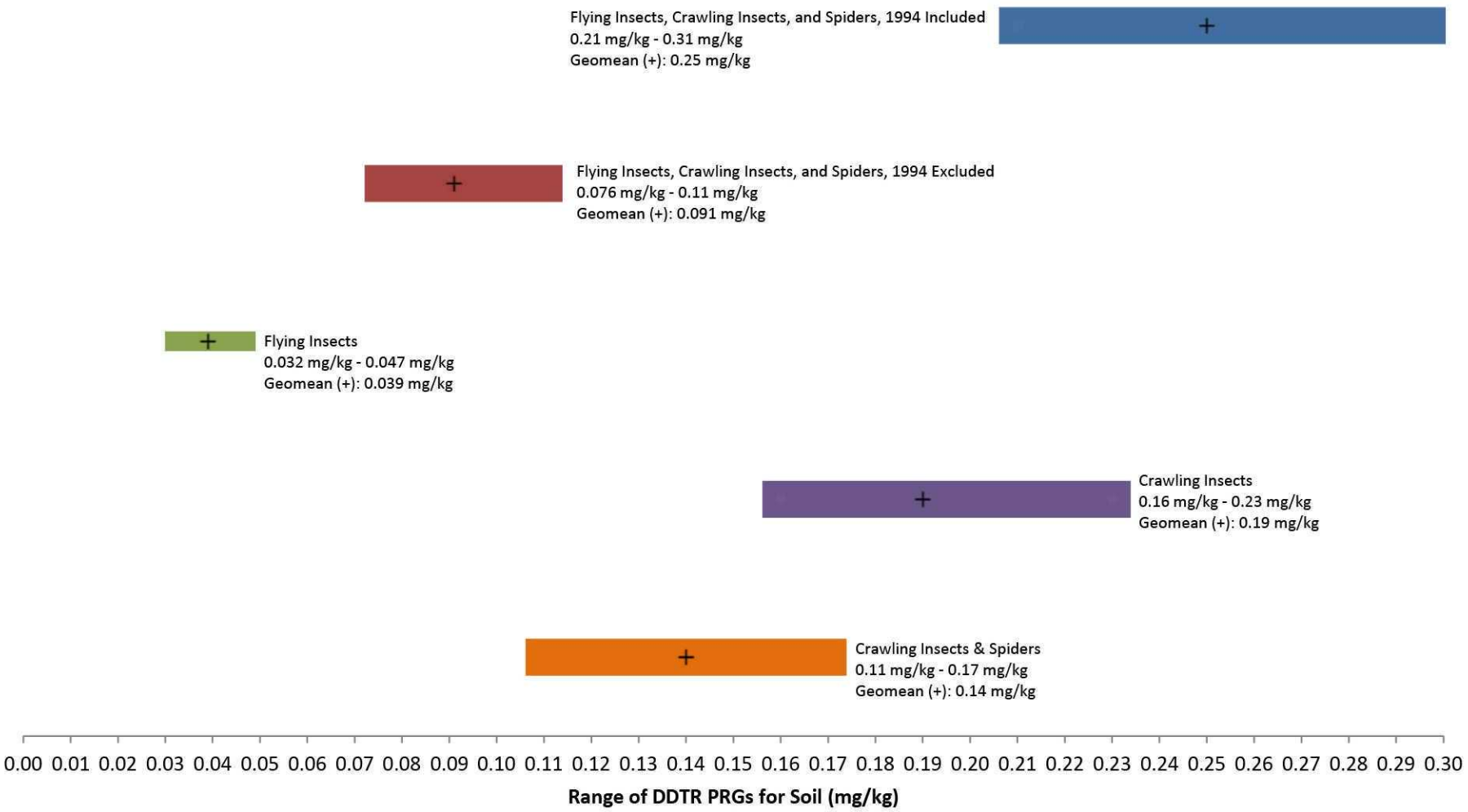
FIGURE 4-2
Mercury Target Soil Concentrations Protective of the Carolina Wren



Note: Values represent NOAEL, LOAEL, and geometric mean PRGs (Table 4-5).

Prepared By: NSR 4/16/12
Checked By: EFC 4/16/12

FIGURE 4-3
DDTR Target Soil Concentrations Protective of the Carolina Wren (Normalized Data)



+ Indicates the geometric mean PRG for the invertebrate grouping (Table 4-6).

Prepared By: NSR 4/16/12
Checked By: EFC 4/16/12

APPENDIX A-1

Aquatic Data Pairings and Regression Plots – Fish Tissue and Sediment

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB	NE Basin	3	NA	NA	ODG0301-0694	113	93	1994	0.84	0.91	OLE0105-0694
1994			NA	NA	ODG0302-0694	81			0.86		OLE0107-0694
			NA	NA	ODG0303-0694	85			0.73		OLE0108-0694
									1.20		OLE0109-0694
Largemouth Bass, WB	NE Basin	19	NA	NA	SGH10-081391	0.39	99	1991	0.84	0.77	LB-E1-03-WB-1191
1991			NA	NA	SGI10-081191	290			0.70		LB-E1-02-WB-1191
			NA	NA	SGG09-080991	31.2					
			NA	NA	SGH09-081091	25.2					
			NA	NA	SGI09-081091	14.8					
			NA	NA	SGJ09-081091	30.9					
			NA	NA	SGG08-081191	30.2					
			NA	NA	SGH08-081191	39					
			NA	NA	SGI08-081391	29					
			NA	NA	SGG07-081391	29.5					
			NA	NA	SGH07-081391	26					
			NA	NA	SGI07-081391	227					
			NA	NA	SCI701-1191	214					
			NA	NA	SCI702-1191	329					
			NA	NA	SGJ07-081191	37.4					
			NA	NA	SGG06-081391	63.7					
			NA	NA	SGH06-081391	200					
			NA	NA	SGI06-081391	137					
			NA	NA	SGJ06-081191	135					
Largemouth Bass, WB	NW Basin	27	NA	NA	SGD11-081391	15.6	22	1994	1.00	0.64	OLE0103-0694
1991, 1994			NA	NA	SGB10-080891	0.095		1991	0.43		CIBA-LB-D1-1991
			NA	NA	SGC10-080891	18.8			0.47		CIBA-LB-D2-1991
			NA	NA	SGD10-080891	30.7			0.93		CIBA-LB-D3-1991
			NA	NA	SGE10-080991	8			0.66		CIBA-LB-D4-1991
			SGF10-080991	25.4	SGF10-080991	26.9 (a)			0.76		CIBA-LB-D5-1991
			SGF10DUP-080991	28.4					0.24		CIBA-LB-D6-1991
			NA	NA	SGB09-081091	13.7					
			NA	NA	SGC09-081091	9.8					
			NA	NA	SGD09-081091	10.7					
			NA	NA	SGE09-081091	7.8					
			NA	NA	SGF09-080991	8.7					

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	*Sediment* Concentration (mg/kg)	*Average Sediment* Concentration (mg/kg)	Fish Year	*Fish Tissue* Concentration (mg/kg)	*Ave. Fish Tissue* Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB	NW Basin	27	NA	NA	SGB08-081391	10.2					
1991, 1994			NA	NA	SGC08-081391	18.8					
(Continued)			NA	NA	SGD08-081391	18.4					
			NA	NA	SGE08-081391	17.4					
			NA	NA	SGF08-080991	4.4					
			NA	NA	SGA07-081391	0.34					
			NA	NA	SGB07-081391	84					
			SGC07-081391	21.3	SGC07-081391	23.1 (a)					
			SGC07DUP-081391	24.8							
			NA	NA	SGD07-081391	12.9					
			NA	NA	SGE07-081391	22.6					
			NA	NA	SGF07-081191	34					
			NA	NA	SGB06-081391	57.8 (b)					
			SGC06-081191	26.9	SGC06-081191	28.4 (a),(b)					
			SGC06DUP-081191	29.9							
			NA	NA	SGD06-081191	22.4 (b)					
			NA	NA	SGE06-081391	17.1 (b)					
			NA	NA	SGF06-081391	79 (b)					
Largemouth Bass, WB	NE/NW Basin	49	NA	NA	ODG0301-0694	113	57	1991	1.2	0.80	LB-G1-37-WB-1191
1991 ,1994			NA	NA	ODG0302-0694	81			0.76		LB-E6-34-WB-1191
			NA	NA	ODG0303-0694	85			0.70		LB-E5-32-WB-1191
			NA	NA	SGH10-081391	0.39			0.76		LB-E5-30-WB-1191
			NA	NA	SGI10-081191	290			0.79		LB-E5-28-WB-1191
			NA	NA	SGG09-080991	31.2			0.47		LB-E3-25-WB-1191
			NA	NA	SGH09-081091	25.2			0.77		LB-E3-23-WB-1191
			NA	NA	SGI09-081091	14.8			0.91		LB-E3-21-WB-1191
			NA	NA	SGJ09-081091	30.9					
			NA	NA	SGG08-081191	30.2					
			NA	NA	SGH08-081191	39					
			NA	NA	SGI08-081391	29					
			NA	NA	SGG07-081391	29.5					
			NA	NA	SGH07-081391	26					
			NA	NA	SGI07-081391	227					
			NA	NA	SCI701-1191	214					
			NA	NA	SCI702-1191	329					

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB	NE/NW Basin	49	NA	NA	SGJ07-081191	37.4					
1991 ,1994			NA	NA	SGG06-081391	63.7					
(Continued)			NA	NA	SGH06-081391	200					
			NA	NA	SGI06-081391	137					
			NA	NA	SGJ06-081191	135					
			NA	NA	SGD11-081391	15.6					
			NA	NA	SGB10-080891	0.095					
			NA	NA	SGC10-080891	18.8					
			NA	NA	SGD10-080891	30.7					
			NA	NA	SGE10-080991	8					
			SGF10-080991	25.4	SGF10-080991	26.9 (a)					
			SGF10DUP-080991	28.4							
			NA	NA	SGB09-081091	13.7					
			NA	NA	SGC09-081091	9.8					
			NA	NA	SGD09-081091	10.7					
			NA	NA	SGE09-081091	7.8					
			NA	NA	SGF09-080991	8.7					
			NA	NA	SGB08-081391	10.2					
			NA	NA	SGC08-081391	18.8					
			NA	NA	SGD08-081391	18.4					
			NA	NA	SGE08-081391	17.4					
			NA	NA	SGF08-080991	4.4					
			NA	NA	SGA07-081391	0.34					
			NA	NA	SGB07-081391	84					
			SGC07-081391	21.3	SGC07-081391	23.1 (a)					
			SGC07DUP-081391	24.8							
			NA	NA	SGD07-081391	12.9					
			NA	NA	SGE07-081391	22.6					
			NA	NA	SGF07-081191	34					
			NA	NA	SGB06-081391	57.8 (b)					
			SGC06-081191	26.9	SGC06-081191	28.4 (a),(b)					
			SGC06DUP-081191	29.9							
			NA	NA	SGD06-081191	22.4 (b)					
			NA	NA	SGE06-081391	17.1 (b)					
			NA	NA	SGF06-081391	79 (b)					

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB 1991, 1994	SW Basin	26	NA	NA	SGB06-081391	57.8 (b)	42.9	1994	0.93	0.93	OLE0102-0694
			SGC06-081191	26.9	SGC06-081191	28.4 (a),(b)					
			SGC06DUP-081191	29.9							
			NA	NA	SGD06-081191	22.4 (b)					
			NA	NA	SGE06-081391	17.1 (b)					
			NA	NA	SGF06-081391	79 (b)					
			NA	NA	SGB05-081391	246					
			NA	NA	SGC05-081391	7.1					
			NA	NA	SGD05-081391	26.2					
			NA	NA	SGE05-081391	97.5					
			NA	NA	SGF05-081391	66.3					
			NA	NA	ODG0101-0694	53					
			NA	NA	ODG0102-0694	62					
			NA	NA	ODG0103-0694	63					
			SGB04-081491	21.6	SGB04-081491	42.3 (a)					
Largemouth Bass, WB 1991, 1994	SW Basin	26	SGB04DUP-081491	62.9							
			NA	NA	SGC04-081491	17					
			NA	NA	SGD04-081491	18.1					
			NA	NA	SGE04-081491	3.2					
			NA	NA	SGF04-081491	12.5					
			NA	NA	SGD03-081491	128					
			NA	NA	SGE03-081491	9.3					
			NA	NA	SGF03-081491	3.7					
			NA	NA	SCE201-1191	5.1					
			NA	NA	SCE202-1191	2.1					
			NA	NA	SGE02-081491	17.4					
			NA	NA	SGF02-081491	27.4					
			NA	NA	SGF01-081491	3.1					

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB	Round Pond	11	NA	NA	ODG0501-0694	26	15	1994	0.49	0.72	OLE0201-0694
1991, 1994			NA	NA	ODG0502-0694	19			1.00		OLE0204-0694
			NA	NA	ODG0503-0694	19			0.68		OLE0206-0694
			NA	NA	SGFP12-083192	8.5					
			NA	NA	SGFP13-083192	6.9					
			NA	NA	SGFP17-083192	22.2					
			NA	NA	SGFP18-083192	10.5					
			NA	NA	SGFP19-083192	1.8					
			NA	NA	SGFP20-083192	15.4					
			NA	NA	SGFP21-083192	1.9					
			NA	NA	SGFP22-083192	32.1					
Largemouth Bass, WB	NE Basin	20	NA	NA	SE-I10-0901	32	88	2001	0.20	0.70	BA-1
2001			NA	NA	SE-C-I10-100101-01	56			0.76		BA-2
			NA	NA	SE-C-I10-100101-02	99			0.47		BA-3
			NA	NA	SE-B1-101101-01	91			1.35		BA-4
			NA	NA	SE-B1-101101-02	67					
			NA	NA	SE-B1-101101-03	78					
			NA	NA	SE-B2-101101-01	130					
			NA	NA	SE-B2-101101-02	150					
			NA	NA	SE-B2-101101-03	110					
			NA	NA	SE-B3-101101-01	140					
			NA	NA	SE-B3-101101-02	93					
			NA	NA	SE-B3-101101-03	96					
			NA	NA	SE-B4-101101-01	110					
			NA	NA	SE-B4-101101-02	110					
			NA	NA	SE-B4-101101-03	130					
			NA	NA	SE-H8-0901	44					
			NA	NA	SE-C-I7-100101-01	68					
			NA	NA	SE-C-I7-100101-02	64					
			NA	NA	SE-H6-0901	42					
			NA	NA	SE-J6-0901	47					

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB	NW Basin	9	NA	NA	SE-B5-101101-01	36	76	2001	1.6	1.5	BA-5
2001			NA	NA	SE-B5-101101-02	51			1.4		BA-10
			NA	NA	SE-B5-101101-03	43					
			NA	NA	SE-B10-101101-01	41					
			NA	NA	SE-B10-101101-02	46					
			SE-B10-101101-03	52	SE-B10-101101-03	66 (a)					
			SE-B10-101101-04 (Dup of SE-B10-101101-03)	86							
			SE-B10-101101-05 (Dup of SE-B10-101101-03)	93							
			SE-B10-101101-06 (Dup of SE-B10-101101-03)	32							
			NA	NA	SE-D10-0901	330					
			NA	NA	SE-F7-0901	42					
			NA	NA	SE-C6-0901	33					
Largemouth Bass, WB	SE Basin	9	NA	NA	SE-G3-0901	4.3	22	2001	1.3	1.3	BA-6
2001			NA	NA	SE-H2-0901	26					
			NA	NA	SE-H4-0901	37					
			NA	NA	SE-J3-0901	30					
			NA	NA	SE-K4-0901	9.1					
			NA	NA	SE-K5-0901	18					
			NA	NA	SE-B6-101101-01	25					
			NA	NA	SE-B6-101101-02	24					
			SE-B6-101101-03	27	SE-B6-101101-03	23 (a)					
			SE-B6-101101-04 (Dup of SE-B6-101101-03)	22							
			SE-B6-101101-05 (Dup of SE-B6-101101-03)	21							
			SE-B6-101101-06 (Dup of SE-B6-101101-03)	22							

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	*Sediment* Concentration (mg/kg)	*Average Sediment* Concentration (mg/kg)	Fish Year	*Fish Tissue* Concentration (mg/kg)	*Ave. Fish Tissue* Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB	Round Pond	10	NA	NA	SE-R1-100401-01	18	21	2001	1.0	0.86	RP-7
2001			NA	NA	SE-R1-100401-02	28			0.60		RP-8
(Continued)			SE-R1-100401-03	27	SE-R1-100401-03	34 (a)			1.0		RP-9
			SE-R1-100401-04 (Dup of SE-R1-100401-03)	28							
			SE-R1-100401-05 (Dup of SE-R1-100401-03)	45							
			SE-R1-100401-06 (Dup of SE-R1-100401-03)	35							
			NA	NA	SE-R2-100401-01	12					
			NA	NA	SE-R2-100401-02	16					
			NA	NA	SE-R2-100401-03	15					
			NA	NA	SE-R7-100401-01	18					
			NA	NA	SE-R7-100401-02	25					
			NA	NA	SE-R7-100401-03	20					
			SE-FP17-0901	24	SE-FP17-0901	26 (a)					
			SE-FP17DUP-0901	27							
Largemouth Bass, WB	NE Basin	7	OU2B-SED-502DC-08	22.4	OU2B-SED-502D-08	93 (c)	41	2008	1.8	1.5	MCI-0021-08WB-NE
2008			OU2B-SED-502DNE-08	213					1.4		MCI-0022-08WB-NE
			OU2B-SED-502DNW-08	59.2					1.4		MCI-0023-08WB-NE
			OU2B-SED-502DSE-08	72					1.8		MCI-0024-08WB-NE
			OU2B-SED-502DSW-08	96.9					1.7		MCI-0043-08WB-NE
			NA	NA	OU2B-SED-404C-08	0.97			1.5		MCI-0054-08WB-NE
			NA	NA	OU2B-SED-403C-08	33			1.3		MCI-0055-08WB-NE
			NA	NA	OU2B-SED-004C-08	38			1.3		MCI-0056-08WB-NE
			OU2B-SED-106C-08	37	OU2B-SED-106C-08	37 (a)			1.3		MCI-0057-08WB-NE
			OU2B-SED-DUP06C-08	36.8					1.4		MCI-0058-08WB-NE
			OU2B-SED-104DC-08	33.5	OU2B-SED-104D-08	51 (c)					
			OU2B-SED-104DNE-08	35.9							
			OU2B-SED-104DNW-08	38.4							
			OU2B-SED-104DSE-08	47							
			OU2B-SED-104DSW-08	99.4							
			NA	NA	OU2B-SED-105C-08	36					

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	*Sediment* Concentration (mg/kg)	*Average Sediment* Concentration (mg/kg)	Fish Year	*Fish Tissue* Concentration (mg/kg)	*Ave. Fish Tissue* Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB 2008	NW Basin	6	NA	NA	OU2B-SED-401C-08	34	24	2008	1.8	1.5	MCI-0025-08WB-NW
			OU2B-SED-501DC-08	18.1	OU2B-SED-501D-08	21 (c)			1.7		MCI-0026-08WB-NW
			OU2B-SED-501DNE-08	27.4					1.2		MCI-0027-08WB-NW
			OU2B-SED-501DNW-08	17.5					1.4		MCI-0028-08WB-NW
			OU2B-SED-501DSE-08	23.4					1.9		MCI-0029-08WB-NW
			OU2B-SED-501DSW-08	18.2					1.3		MCI-0044-08WB-NW
			NA	NA	OU2B-SED-402C-08	18			1.2		MCI-0045-08WB-NW
			NA	NA	OU2B-SED-101C-08	22			1.5		MCI-0046-08WB-NW
			OU2B-SED-102C-08	26.5	OU2B-SED-102C-08	26 (a)			1.7		MCI-0047-08WB-NW
			OU2B-SED-DUP01C-08 (Dup of OU2B-SED-102C-08)	26.0					1.4		MCI-0048-08WB-NW
			OU2B-SED-103DC-08	25.9	OU2B-SED-103D-08	26 (c)					
			OU2B-SED-103DNE-08	24.6							
			OU2B-SED-103DNW-08	25.3							
			OU2B-SED-103DSE-08	26.3							
			OU2B-SED-103DSW-08	26.5							
Largemouth Bass, WB 2008	SE Basin	4	OU2B-SED-303DC-08	19.8	OU2B-SED-303D-08	22 (c)	32	2008	1.4	1.5	MCI-0035-08WB-SE
			OU2B-SED-DUP05C-08 (Dup of OU2B-SED-303DC-08)	16.3					1.4		MCI-0036-08WB-SE
			OU2B-SED-303DNE-08	19.8					1.2		MCI-0037-08WB-SE
			OU2B-SED-303DNW-08	22.8					1.8		MCI-0038-08WB-SE
			OU2B-SED-303DSE-08	37.0					1.5		MCI-0039-08WB-SE
			OU2B-SED-303DSW-08	18.3					1.5		MCI-0040-08WB-SE
			OU2B-SED-204C-08	93.2	OU2B-SED-204C-08	71.7 (a)			1.4		MCI-0041-08WB-SE
			OU2B-SED-DUP03C-08 (Dup of OU2B-SED-204C-08)	50.1							
			NA	NA	OU2B-SED-304C-08	25			1.6		MCI-0042-08WB-SE
			NA	NA	OU2B-SED-205C-08	8.0			1.1		MCI-0059-08WB-SE
			NA	NA					1.6		MCI-0060-08WB-SE

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB 2008	SW Basin	5	OU2B-SED-201C-08	64	OU2B-SED-201C-08	50 (a)	40	2008	2.0	1.7	MCI-0030-08WB-SW
			OU2B-SED-DUP02C-08 (Dup of OU2B-SED-201C-08)	36.6					1.6		MCI-0031-08WB-SW
			OU2B-SED-202DC-08	80	OU2B-SED-202D-08	104 (c)			1.8		MCI-0032-08WB-SW
			OU2B-SED-202DNE-09	100					1.9		MCI-0033-08WB-SW
			OU2B-SED-202DNW-10	172					1.6		MCI-0034-08WB-SW
			OU2B-SED-202DSE-11	139					1.5		MCI-0049-08WB-SW
			OU2B-SED-202DSW-12	31					1.6		MCI-0050-08WB-SW
			NA	NA	OU2B-SED-301C-08	5.8			1.8		MCI-0051-08WB-SW
			OU2B-SED-302C-08	3.46	OU2B-SED-302C-08	3.35 (a)			1.6		MCI-0052-08WB-SW
			OU2B-SED-DUP04C-08 (Dup of OU2B-SED-302C-08)	3.24							
			OU2B-SED-203DC-08	37.8	OU2B-SED-203D-08	36 (c)			1.5		MCI-0053-08WB-SW
			OU2B-SED-203DNE-08	37.6							
			OU2B-SED-203DNW-08	37.0							
			OU2B-SED-203DSE-08	34.8							
			OU2B-SED-203DSW-08	31.7							
Largemouth Bass, WB 1994	Reference Area Stimpson Wildlife Sanctuary	12	NA	NA	RDG0201	0.031	0.063	1994	0.18	0.21	RLE0101
			NA	NA	RDG0202	0.050			0.13		RLE0102
			NA	NA	RDG0203	0.053			0.16		RLE0103
			NA	NA	RDG0301	0.069			0.15		RLE0104
			NA	NA	RDG0302	0.085			0.34		RLE0105

TABLE A-1

Data Pairing for Mercury in Predatory Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Largemouth Bass, WB 1994 (Continued)	Reference Area Stimpson Wildlife Sanctuary	12	NA	NA	RDG0303	0.072		1994	0.19		RLE0106
			NA	NA	RDG0401	0.077			0.14		RLE0107
			NA	NA	RDG0402	0.080			0.21		RLE0108
			NA	NA	RDG0403	0.077			0.36		RLE0109
			NA	NA	RDG0601	0.045					
			NA	NA	RDG0602	0.061					
			NA	NA	RDG0603	0.052					
Largemouth Bass, WB 1991	Reference Area Ciba	3	NA	NA	CIBA-BG1-1991	0.08	0.06	1991	0.22	0.23	CIBA-LB-BG1-1991
			NA	NA	CIBA-BG2-1991	0.07			0.27		CIBA-LB-BG2-1991
			NA	NA	CIBA-BG3-1991	0.02			0.20		CIBA-LB-BG3-1991
Largemouth Bass, WB 1992	Reference Area Tombigbee River	1	NA	NA	SGTR01-090392	0.39	0.39	1993	0.10	0.17	MT-7SL-3354
									0.03		MT-7ML-3352
									0.13		MT-7ML-3350
									0.13		MT-7LL-3348
									0.44		MT-7LL-3346
Largemouth Bass, WB 1994	Reference Area Three Rivers Lake	3	NA	NA	MT-8(A)-85042	0.16	0.19	1994	0.09	0.11	MT-8SL-3387
			NA	NA	MT-8(B)-85043	0.21			0.13		MT-8LL-3385
			NA	NA	MT-8(C) -85044	0.20					
Largemouth Bass, WB 1994	Reference Area Tensaw Lake	4	NA	NA	MT-11(A)-85066	0.20	0.19	1994	0.18	0.22	MT-11SL-3393
			NA	NA	MT-11(B)-85067	0.19			0.25		MT-11SL-3395
			NA	NA	MT-11 (C) -85068	0.17			0.24		MT-11SL-3397
			NA	NA	MT-11(D)-85069	0.18					

Notes:

(a) Sediment concentration is the average of the parent sample and the duplicate sample.

(b) Sediment sample located on the dividing line between the northwest and southwest basin. Sample included in both quadrants.

(c) Sediment concentration is the average of a 5-point composite sample.

WB = Whole Body

NW = Northwest

NE = Northeast

SW = Southwest

SE = Southeast

NA = Not Applicable

Prepared/Date: MKB 3/17/11

Checked/Date: HEF 3/25/11

Revised/Date: NSR 12/19/11

Checked/Date: EFC 12/20/11

TABLE A-2

Data Pairing for Mercury in Forage Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Mosquitofish, WB 1991, 1994	NE Basin	15	NA	NA	ODG0301-0694	113	114	1994	0.5	0.45	OGS0101-0694
			NA	NA	ODG0302-0694	81			0.41		OGS0102-0694
			NA	NA	ODG0303-0694	85			0.44		OGS0103-0694
			NA	NA	SGI08-081391	29					
			NA	NA	SCI701-1191	214					
			NA	NA	SCI702-1191	329					
			NA	NA	SCI703-1191	214					
			NA	NA	SGI07-081391	227					
			NA	NA	SGJ07-081191	37.4					
			NA	NA	SGH07-081391	26					
			NA	NA	SGH08-081191	39					
			NA	NA	SGI06-081391	137					
			NA	NA	SGI09-081091	14.8					
			NA	NA	SGJ06-081191	135					
			NA	NA	SGJ09-081091	30.9					
Mosquitofish, WB 1991, 1994	Round Pound	11	NA	NA	ODG0501-0694	26	15	1994	0.28	0.275	OGS0308-0694
			NA	NA	ODG0502-0694	19			0.27		OGS0309-0694
			NA	NA	ODG0503-0694	19					
			NA	NA	SGFP12-083192	8.5					
			NA	NA	SGFP13-083192	6.9					
			NA	NA	SGFP17-083192	22.2					
			NA	NA	SGFP18-083192	10.5					
			NA	NA	SGFP19-083192	1.8					
			NA	NA	SGFP20-083192	15.4					
			NA	NA	SGFP21-083192	1.9					
			NA	NA	SGFP22-083192	32.1					
Mosquitofish, WB 2001	NE Basin	13	NA	NA	SE-B1-101101-01	91	91	2001	0.49	0.47	GB-B1-100101-01A
			NA	NA	SE-B1-101101-02	67			0.48		GB-B1-100101-01B
			NA	NA	SE-B1-101101-03	78			0.45		GB-B1-100101-01C
			NA	NA	SE-B2-101101-01	130					
			NA	NA	SE-B2-101101-02	150					
			NA	NA	SE-B2-101101-03	110					
			NA	NA	SE-C-I10-100101-01	56					
			NA	NA	SE-C-I10-100101-02	99					
			NA	NA	SE-I10-0901	32					
			NA	NA	SE-B3-101101-01	140					
			NA	NA	SE-B3-101101-02	93					
			NA	NA	SE-B3-101101-03	96					
			NA	NA	SE-H8-0901	44					
Mosquitofish, WB 2001	NE Basin	15	NA	NA	SE-B2-101101-01	130	99	2001	0.48	0.46	GB-B2-100101-02A
			NA	NA	SE-B2-101101-02	150			0.41		GB-B2-100101-02B
			NA	NA	SE-B2-101101-03	110			0.50		GB-B2-100101-02C
			NA	NA	SE-B3-101101-01	140					
			NA	NA	SE-B3-101101-02	93					
			NA	NA	SE-B3-101101-03	96					
			NA	NA	SE-C-I10-100101-01	56					
			NA	NA	SE-C-I10-100101-02	99					
			NA	NA	SE-I10-0901	32					
			NA	NA	SE-B1-101101-01	91					
			NA	NA	SE-B1-101101-02	67					
			NA	NA	SE-B1-101101-03	78					

TABLE A-2

Data Pairing for Mercury in Forage Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Mosquitofish, WB 2001 (continued)	NE Basin	15	NA	NA	SE-B4-101101-01	110					
			NA	NA	SE-B4-101101-02	110					
			NA	NA	SE-B4-101101-03	130					
Mosquitofish, WB 2001	NE Basin	12	NA	NA	SE-B4-101101-01	110	105	2001	0.42	0.44	GB-B4-100101-03A
			NA	NA	SE-B4-101101-02	110			0.47		GB-B4-100101-03B
			NA	NA	SE-B4-101101-03	130			0.44		GB-B4-100101-03C
			NA	NA	SE-B3-101101-01	140					
			NA	NA	SE-B3-101101-02	93					
			NA	NA	SE-B3-101101-03	96					
			NA	NA	SE-B2-101101-01	130					
			NA	NA	SE-B2-101101-02	150					
			NA	NA	SE-B2-101101-03	110					
			NA	NA	SE-C-I10-100101-01	56					
			NA	NA	SE-C-I10-100101-02	99					
			NA	NA	SE-I10-0901	32					
Mosquitofish, WB 2001	SE Basin	5	NA	NA	SE-B6-101101-01	25	26	2001	0.19	0.38	GB-B6-100201-06A
			NA	NA	SE-B6-101101-02	24			0.47		GB-B6-100201-06B
			SE-B6-101101-03	27	SE-B6-101101-03	23 (a)			0.49		GB-B6-100201-06C
			SE-B6-101101-04 (Dup of SE-B6-101101-03)	22							
			SE-B6-101101-05 (Dup of SE-B6-101101-03)	21							
			SE-B6-101101-06 (Dup of SE-B6-101101-03)	22							
			NA	NA	SE-J3-0901	30					
			NA	NA	SE-H2-0901	26					
Mosquitofish, WB 2001	NW Basin	4	NA	NA	SE-B10-101101-01	41	121	2001	0.44	0.47	GB-B10-100201-07A
			NA	NA	SE-B10-101101-02	46			0.51		GB-B10-100201-07B
			SE-B10-101101-03	52	SE-B10-101101-03	66 (a)			0.45		GB-B10-100201-07C
			SE-B10-101101-04 (Dup of SE-B10-101101-03)	86							
			SE-B10-101101-05 (Dup of SE-B10-101101-03)	93							
			SE-B10-101101-06 (Dup of SE-B10-101101-03)	32							
			NA	NA	SE-D10-0901	330					
Mosquitofish, WB 2001	Round Pound	10	NA	NA	SE-R1-100401-01	18	21	2001	0.4	0.41	GB-R1-100201-04A
			NA	NA	SE-R1-100401-02	28			0.41		GB-R1-100201-04B
			SE-R1-100401-03	27	SE-R1-100401-03	34 (a)			0.42		GB-R1-100201-04C
			SE-R1-100401-04 (Dup of SE-R1-101101-03)	28							
			SE-R1-100401-05 (Dup of SE-R1-101101-03)	45							
			SE-R1-100401-06 (Dup of SE-R1-101101-03)	35							
			NA	NA	SE-R2-100401-01	12					
			NA	NA	SE-R2-100401-02	16					
			NA	NA	SE-R2-100401-03	15					
			NA	NA	SE-R7-100401-01	18					
			NA	NA	SE-R7-100401-02	25					

TABLE A-2

Data Pairing for Mercury in Forage Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Mosquitofish, WB 2001 (continued)	Round Pound	10	NA	NA	SE-R7-100401-03	20					
			SE-FP17-0901	24	SE-FP17-0901	26 (a)					
			SE-FP17DUP-0901	27							
Mosquitofish, WB 2001	Round Pound	10	NA	NA	SE-R1-100401-01	18	21	2001	0.47	0.37	GB-R2-100201-05A
			NA	NA	SE-R1-100401-02	28			0.43		GB-R2-100201-05B
			SE-R1-100401-03	27	SE-R1-100401-03	34 (a)			0.21		GB-R2-100201-05C
			SE-R1-100401-04 (Dup of SE-R1-101101-03)	28							
			SE-R1-100401-05 (Dup of SE-R1-101101-03)	45							
			SE-R1-100401-06 (Dup of SE-R1-101101-03)	35							
			NA	NA	SE-R2-100401-01	12					
			NA	NA	SE-R2-100401-02	16					
			NA	NA	SE-R2-100401-03	15					
			NA	NA	SE-R7-100401-01	18					
			NA	NA	SE-R7-100401-02	25					
			NA	NA	SE-R7-100401-03	20					
			SE-FP17-0901	24	SE-FP17-0901	26 (a)					
			SE-FP17DUP-0901	27							
Silverside, Comp 2008	NE Basin	3	NA	NA	OU2B-SED-404C-08	0.97	42	2008	0.6	0.9	MCI-0081-08WB-NE
			OU2B-SED-502DC-08	22.4	OU2B-SED-502D-08	93 (b)			1.2		MCI-0082-08WB-NE
			OU2B-SED-502DNE-08	213							
			OU2B-SED-502DNW-08	59.2							
			OU2B-SED-502DSE-08	72							
			OU2B-SED-502DSW-08	96.9							
			NA	NA	OU2B-SED-403C-08	33.1					
Silverside, Comp 2008	SE Basin	1	NA	NA	OU2B-SED-304C-08	25	25	2008	0.82	0.82	MCI-0083-08WB-SE
			NA	NA							
Silverside, Comp 2008	NW Basin	2	NA	NA	OU2B-SED-101C-08	21.8	28	2008	0.82	0.82	MCI-0085-08WB-NW
			NA	NA	OU2B-SED-401C-08	33.6					
Silverside, Comp 2008	SW Basin	2	OU2B-SED-201C-08	64	OU2B-SED-201C-08	50 (a)	28	2008	0.74	0.74	MCI-0084-08WB-SW
			OU2B-SED-DUP02C-08 (Dup of OU2B-SED-201C-08)	36.6							
			NA	NA	OU2B-SED-301C-08	5.82					
Bluegill, WB 2008	NW Basin	2	NA	NA	OU2B-SED-101C-08	21.8	28	2008	0.85	0.684	MCI-0066-08WB-NW
			NA	NA	OU2B-SED-401C-08	33.6			0.57		MCI-0067-08WB-NW
			NA	NA					0.63		MCI-0068-08WB-NW
			NA	NA					0.58		MCI-0069-08WB-NW
			NA	NA					0.79		MCI-0070-08WB-NW
Bluegill, WB - 2008	NE Basin	3	NA	NA	OU2B-SED-404C-08	0.97	42	2008	0.63	0.702	MCI-0061-08WB-NE
			OU2B-SED-502DC-08	22.4	OU2B-SED-502D-08	93 (b)			0.54		MCI-0062-08WB-NE
			OU2B-SED-502DNE-08	213					0.84		MCI-0063-08WB-NE
			OU2B-SED-502DNW-08	59.2					0.70		MCI-0064-08WB-NE
			OU2B-SED-502DSE-08	72					0.80		MCI-0065-08WB-NE
			OU2B-SED-502DSW-08	96.9							
			NA	NA	OU2B-SED-403C-08	33.1					

TABLE A-2

Data Pairing for Mercury in Forage Fish
OLIN McINTOSH OU-2

Matrix	Area	Number Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs	Sediment Concentration (mg/kg)	Average Sediment Concentration (mg/kg)	Fish Year	Fish Tissue Concentration (mg/kg)	Ave. Fish Tissue Concentration (mg/kg)	Fish Sample IDs
Bluegill, WB	SE Basin	1	NA	NA	OU2B-SED-304C-08	25	25	2008	0.66	0.66	MCI-0071-08WB-NW
2008									0.59		MCI-0072-08WB-NW
									0.83		MCI-0073-08WB-NW
									0.61		MCI-0074-08WB-NW
									0.59		MCI-0075-08WB-NW
Bluegill, WB	SW Basin	2	OU2B-SED-201C-08	64	OU2B-SED-201C-08	50 (a)	28	2008	0.59	0.78	MCI-0076-08WB-NW
2008			OU2B-SED-DUP02C-08 (Dup of OU2B-SED-201C-08)	37					0.57		MCI-0077-08WB-NW
			NA	NA	OU2B-SED-301C-08	5.82			0.59		MCI-0078-08WB-NW
									0.94		MCI-0079-08WB-NW
									1.2		MCI-0080-08WB-NW
Mosquitofish, WB - 1994	Reference	12	NA	NA	RDG0201	0.031	0.063	1994	0.080	0.084	RGS0101
	Stimpson		NA	NA	RDG0202	0.05			0.080		RGS0102
	Wildlife Sanctuary		NA	NA	RDG0203	0.053			0.100		RGS0103
			NA	NA	RDG0301	0.069			0.100		RGS0104
			NA	NA	RDG0302	0.085			0.100		RGS0105
			NA	NA	RDG0303	0.072			0.140		RGS0106
			NA	NA	RDG0401	0.077			0.100		RGS0207
			NA	NA	RDG0402	0.08			0.100		RGS0208
			NA	NA	RDG0403	0.077			0.080		RGS0209
			NA	NA	RDG0601	0.045			0.040		RGS0410
			NA	NA	RDG0602	0.061			0.050		RGS0111
			NA	NA	RDG0603	0.052			0.040		RGS0112
Forage Fish, WB	Reference	3	NA	NA	MT-8(A)-85042	0.16	0.19	1994	0.05	0.05	MT-8 FOR
1994	Three Rivers Lake		NA	NA	MT-8(B)-85043	0.21					
			NA	NA	MT-8(C) -85044	0.20					
Forage Fish, WB	Reference	4	NA	NA	MT-11(A)-85066	0.20	0.19	1994	0.10	0.10	MT-11 FOR
1994	Tensaw Lake		NA	NA	MT-11(B)-85067	0.19					
			NA	NA	MT-11 (C) -85068	0.17					
			NA	NA	MT-11(D)-85069	0.18					

Notes:
(a) Sediment concentration is the average of the parent sample and the duplicate sample.
(b) Sediment concentration is the average of a 5-point composite sample.
WB = Whole Body
Comp = Composite Sample
NW = Northwest
NE = Northeast
SW = Southwest
SE = Southeast
NA = Not Applicable

Prepared/Date: MKB 3/17/11
Checked/Date: HEF 3/25/11
Revised/Date: NSR 12/21/11
Checked/Date: MKB 01/05/12

TABLE A-3

Data Pairing for DDTR in Forage Fish
OLIN McINTOSH OU-2

Matrix	Area	Number of Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs (a)	Sediment Concentration (mg/kg)	Ave. Sediment Concentration (mg/kg)	TOC (mg/kg)	FOC	Avg Sed. Conc./Avg FOC (mg/kg Organic Carbon)	Fish Year	Tissue Concentration (mg/kg)	Fraction Lipids	Norm. Fish Tissue Concentration (mg DDTR/kg lipid)	Ave. Norm. Fish Tissue Concentration (mg DDTR/kg lipid)	Fish Sample IDs
Mosquitofish, WB 1991, 1994	NE Basin	6	NA	NA	ODG0301-0694	4.75	3.29	16000	0.016	107	1994	4.50	0.045	101	85	OGS0101-0694
			NA	NA	ODG0302-0694	5.28						4.21	0.044	95		OGS0102-0694
			NA	NA	ODG0303-0694	6.18						4.46	0.074	60		OGS0103-0694
			NA	NA	SGI08-081391	NA										
			NA	NA	SCI701-1191	NA										
			NA	NA	SCI702-1191	NA										
			NA	NA	SGI07-081391	NA										
			NA	NA	SGJ07-081191	1.7		36900	0.0369							
			NA	NA	SGH07-081391	NA										
			NA	NA	SGH08-081191	1.36										
			NA	NA	SGI06-081391	NA										
			NA	NA	SGI09-081091	NA										
			NA	NA	SGJ06-081191	0.494		39400	0.0394							
			NA	NA	SGJ09-081091	NA										
Mosquitofish, WB 1994	Round Pond	3	NA	NA	ODG0501-0694	5.86	6.33	16000	0.016	396	1994	14.9	0.048	311	290	OGS0308
			NA	NA	ODG0502-0694	5.99						14.9	0.055	270		OGS0309
			NA	NA	ODG0503-0694	7.14										
Mosquitofish, WB 2001	NW Basin	4	NA	NA	SE-B10-101101-01	4.52	2.66	65000	0.065	63	2001	1.59	0.0281	57	57	GB-B10-100201-07A
			NA	NA	SE-B10-101101-02	2.50						1.88	0.0307	61		GB-B10-100201-07B
			SE-B10-101101-03	2.33	SE-B10-101101-03	2.44 (a)						1.78	0.0336	53		GB-B10-100201-07C
			SE-B10-101101-04 (Dup of SE-B10-101101-03)	3.78				32000	0.032							
			SE-B10-101101-05 (Dup of SE-B10-101101-03)	1.96												
			SE-B10-101101-06 (Dup of SE-B10-101101-03)	1.70												
			NA	NA	SE-D10-0901	1.20		29000	0.029							
Mosquitofish, WB 2001	NE Basin	11	NA	NA	SE-B1-101101-01	3.39	4.16	84000	0.084	50	2001	1.61	0.0348	46	50	GB-B1-100101-01A
			NA	NA	SE-B1-101101-02	2.73						1.59	0.0346	46		GB-B1-100101-01B
			NA	NA	SE-B1-101101-03	3.34						2.05	0.0352	58		GB-B1-100101-01C
			NA	NA	SE-B2-101101-01	7.64										
			NA	NA	SE-B2-101101-02	6.47										
			NA	NA	SE-B2-101101-03	5.41										
			NA	NA	SE-C-I10-100101-01	NA										
			NA	NA	SE-C-I10-100101-02	NA										
			NA	NA	SE-I10-0901	0.66										
			NA	NA	SE-B3-101101-01	4.61										
			NA	NA	SE-B3-101101-02	5.49										
			NA	NA	SE-B3-101101-03	5.40										
			NA	NA	SE-H8-0901	0.65										
Mosquitofish, WB 2001	NE Basin	13	NA	NA	SE-B2-101101-01	7.64	5.00	140000	0.14	45	2001	1.22	0.0362	34	35.0	GB-B2-100101-02A
			NA	NA	SE-B2-101101-02	6.47						1.27	0.0324	39		GB-B2-100101-02B
			NA	NA	SE-B2-101101-03	5.41						1.40	0.0434	32		GB-B2-100101-02C
			NA	NA	SE-B3-101101-01	4.61		170000	0.17							
			NA	NA	SE-B3-101101-02	5.49										
			NA	NA	SE-B3-101101-03	5.40										
			NA	NA	SE-I10-0901	0.661		24000	0.024							
			NA	NA	SE-C-I10-100101-01	NA										
			NA	NA	SE-C-I10-100101-02	NA										
			NA	NA	SE-B1-101101-01	3.390										
			NA	NA	SE-B1-101101-02	2.730										
			NA	NA	SE-B1-101101-03	3.340										
			NA	NA	SE-B4-101101-01	4.660										
			NA	NA	SE-B4-101101-02	8.990										
			NA	NA	SE-B4-101101-03	6.240										

TABLE A-3

Data Pairing for DDTR in Forage Fish
OLIN McINTOSH OU-2

Matrix	Area	Number of Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs (a)	Sediment Concentration (mg/kg)	Ave. Sediment Concentration (mg/kg)	TOC (mg/kg)	FOC		Avg Sed. Conc./Avg FOC (mg/kg Organic Carbon)	Fish Year	Tissue Concentration (mg/kg)	Fraction Lipids	Norm. Fish Tissue Concentration (mg DDTR/kg lipid)	Ave. Norm. Fish Tissue Concentration (mg DDTR/kg lipid)	Fish Sample IDs
Mosquitofish, WB 2001	NE Basin	10	NA	NA	SE-B4-101101-01	4.66	5.56	130000	0.13		43	2001	1.21	0.0281	43	36	GB-B4-100101-03A
			NA	NA	SE-B4-101101-02	8.99							1.05	0.0307	34		GB-B4-100101-03B
			NA	NA	SE-B4-101101-03	6.24							0.99	0.0336	29		GB-B4-100101-03C
			NA	NA	SE-B3-101101-01	4.61											
			NA	NA	SE-B3-101101-02	5.49											
			NA	NA	SE-B3-101101-03	5.40											
			NA	NA	SE-B2-101101-01	7.64											
			NA	NA	SE-B2-101101-02	6.47											
			NA	NA	SE-B2-101101-03	5.41											
			NA	NA	SE-C-I10-100101-01	NA											
			NA	NA	SE-C-I10-100101-02	NA											
			NA	NA	SE-I10-0901	0.66											
Mosquitofish, WB 2001	SE Basin	5	NA	NA	SE-B6-101101-01	1.01	1.31	25000	0.025		61	2001	1.310	0.0300	44	46	GB-B6-100201-06A
			NA	NA	SE-B6-101101-02	1.00							1.44	0.0320	45		GB-B6-100201-06B
			SE-B6-101101-03	0.89	SE-B6-101101-03	1.00 (a)							1.29	0.0255	50		GB-B6-100201-06C
			SE-B6-101101-04 (Dup of SE-B6-101101-03)	0.91													
			SE-B6-101101-05 (Dup of SE-B6-101101-03)	1.28													
			SE-B6-101101-06 (Dup of SE-B6-101101-03)	0.93													
			NA	NA	SE-J3-0901	1.70		11000	0.011								
			NA	NA	SE-H2-0901	1.82		28000	0.028								
Mosquitofish, WB 2001	Round Pond	10	NA	NA	SE-R1-100401-01	10.2	6.5	120000	0.12	(a)	125	2001	9.64	0.0443	218	291	GB-R1-100201-04A
			NA	NA	SE-R1-100401-02	20.6							10.2	0.0319	320		GB-R1-100201-04B
			SE-R1-100401-03	13.8	SE-R1-100401-03	16.2 (a)							10.8	0.0324	334		GB-R1-100201-04C
			SE-R1-100401-04 (Dup of SE-R1-100401-03)	26.0				110000									
			SE-R1-100401-05 (Dup of SE-R1-100401-03)	10.3													
			SE-R1-100401-06 (Dup of SE-R1-100401-03)	14.7													
			NA	NA	SE-R2-100401-01	2.36		25000	0.025								
			NA	NA	SE-R2-100401-03	2.24											
			NA	NA	SE-R2-100401-03	2.98											
			NA	NA	SE-R7-100401-01	2.84		23000	0.023								
			NA	NA	SE-R7-100401-02	2.73											
			NA	NA	SE-R7-100401-03	2.20											
			SE-FP17-0901	3.4	SE-FP17-0901	2.7 (a)		48000	0.045	(a)							
			SE-FP17DUP-0901	1.9				41000									
Mosquitofish, WB 2001	Round Pond	10	NA	NA	SE-R1-100401-01	10.2	6.5	120000	0.12	(a)	125	2001	6.56	0.034	194	183	GB-R2-100201-05A
			NA	NA	SE-R1-100401-02	20.6							6.54	0.040	164		GB-R2-100201-05B
			SE-R1-101101-03	13.8	SE-R1-100401-03	16.2 (a)							6.81	0.036	191		GB-R2-100201-05C
			SE-R1-101101-04 (Dup of SE-R1-101101-03)	26.0				110000									
			SE-R1-101101-05 (Dup of SE-R1-101101-03)	10.3													
			SE-R1-101101-06 (Dup of SE-R1-101101-03)	14.7													
			NA	NA	SE-R2-100401-01	2.36		25000	0.025								
			NA	NA	SE-R2-100401-02	2.97											
			NA	NA	SE-R2-100401-03	2.23											
			NA	NA	SE-R7-100401-01	2.84		23000	0.023								
			NA	NA	SE-R7-100401-02	2.73											
			NA	NA	SE-R7-100401-03	2.20											
			SE-FP17-0901	3.4	SE-FP17-0901	2.7 (a)		48000	0.045	(a)							
			SE-FP17DUP-0901	1.9				41000									

TABLE A-3

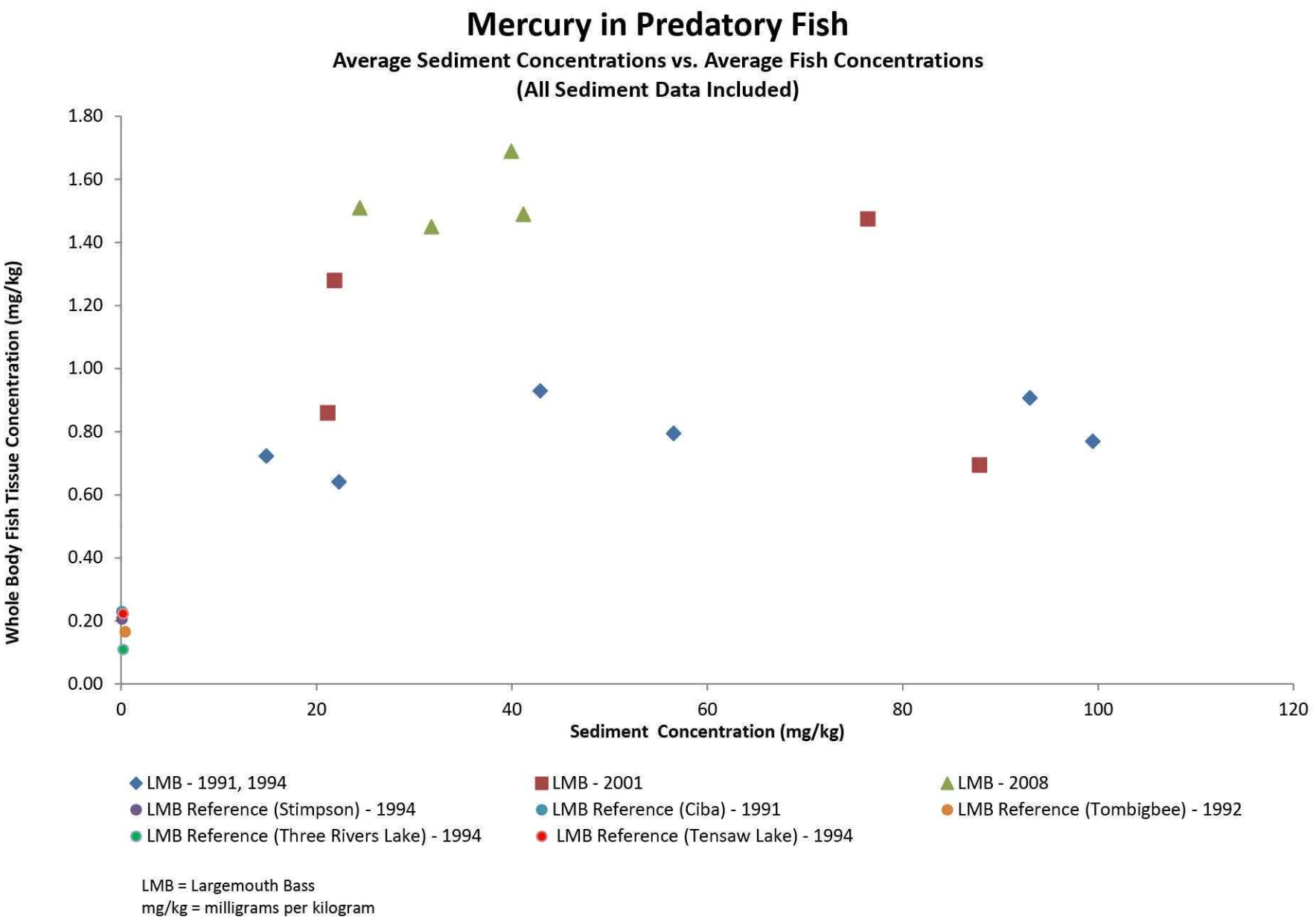
Data Pairing for DDTR in Forage Fish
OLIN McINTOSH OU-2

Matrix	Area	Number of Sediment Samples	Individual Sample IDs for Averaged Samples	Individual Sediment Concentration for Averaged Samples (mg/kg)	Sediment Sample IDs (a)	Sediment Concentration (mg/kg)	Ave. Sediment Concentration (mg/kg)	TOC (mg/kg)	FOC	Avg Sed. Conc./Avg FOC (mg/kg Organic Carbon)	Fish Year	Tissue Concentration (mg/kg)		Fraction Lipids	Norm. Fish Tissue Concentration (mg DDTR/kg lipid)	Ave. Norm. Fish Tissue Concentration (mg DDTR/kg lipid)	Fish Sample IDs
Mosquitofish, WB 1994	Reference Stimpson Wildlife Sanctuary	12	NA	NA	RDG0201	0.000690	0.00481	16000	0.014	0.33	1994	0.072		0.036	2.000	1.88	RGS0101
			NA	NA	RDG0202	0.00867						0.072		0.038	1.885		RGS0102
			NA	NA	RDG0203	0.00493						0.078		0.036	2.173		RGS0103
			NA	NA	RDG0301	0.00453		16000				0.081		0.039	2.066		RGS0104
			NA	NA	RDG0302	0.00433						0.093		0.035	2.688		RGS0105
			NA	NA	RDG0303	0.00146						0.030		0.059	0.505		RGS0106
			NA	NA	RDG0401	0.00433		16000				0.042		0.026	1.622		RGS0207
			NA	NA	RDG0402	0.00611						0.075		0.029	2.560		RGS0208
			NA	NA	RDG0403	0.00335						0.030		0.024	1.255		RGS0209
			NA	NA	RDG0601	0.00236		9470				0.0585		0.033	1.800		RGS0410
			NA	NA	RDG0602	0.00847						0.065		0.032	2.038		RGS0411
			NA	NA	RDG0603	0.00847						0.0635		0.032	1.966		RGS0412
Forage Fish, WB 1994	Reference Three Rivers Lake	3	NA	NA	MT-8(A)-85042	0.154 (b)	0.156			1.33	1994	2.25	(b)	0.087	25.9	25.9	MT-8 FOR
			NA	NA	MT-8(B)-85043	0.148 (b)											
			NA	NA	MT-8(C) -85044	0.165 (b)		NA	0.12								
Forage Fish, WB 1994	Reference Tensaw Lake	4	NA	NA	MT-11(A)-85066	0.154 (b)	0.164			1.33	1994	0.0571	(b)	0.0731	0.782	0.782	MT-11 FOR
			NA	NA	MT-11(B)-85067	0.152 (b)											
			NA	NA	MT-11 (C) -85068	0.175 (b)		NA	0.12								
			NA	NA	MT-11(D)-85069	0.173 (b)											

Notes:
(a) Sediment concentration is the average of the parent sample and the duplicate sample.
(b) Concentration is the calculated DDTR concentration; only the 4,4-DDT, DDE, and DDD isomers data are available. The 4,4-isomer data were multiplied by 1.97 (a factor based on the sediment ratio of 2,4 to 4,4 DDT, DDE and DDD isomers) to generate the DDTR value for each sample. Half the detection limit was used for the non-detect isomers.
WB = Whole Body
NW = Northwest
NE = Northeast
SW = Southwest
SE = Southeast
NA = Not Applicable
TOC = Total Organic Carbon
FOC = Fraction Organic Carbon
(a) Includes only those samples with available sediment TOC data.

Prepared/Date: MKB 3/17/11
Checked/Date: HEF 3/25/11
Revised/Date: NSR 12/21/11
Checked/Date: MKB 01/05/12

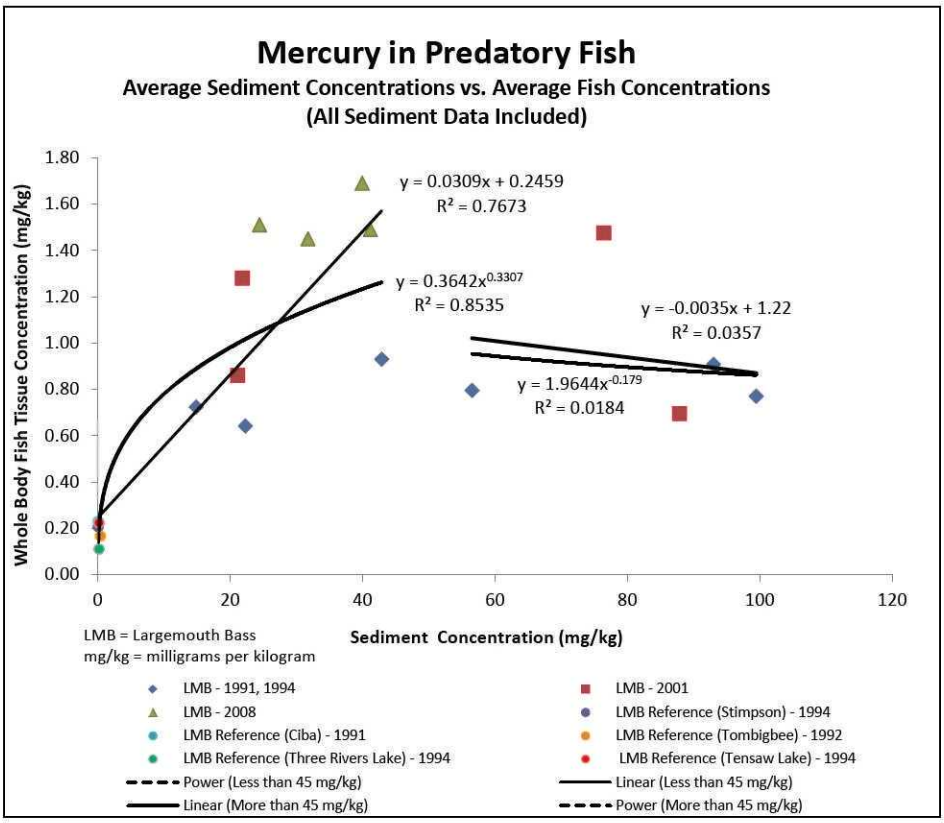
FIGURE A-1a



LMB = Largemouth Bass
mg/kg = milligrams per kilogram

REVISED BY/DATE: NSR 12/19/11
CHECKED BY/DATE: MKB 12/20/11

FIGURE A-1b



SUMMARY OUTPUT

Prepared/Date: LSV 1/27/12
Checked/Date: MKB 1/30/12

Regression Statistics	
Multiple R	0.188898559
R Square	0.035682666
Adjusted R Square	-0.285756446
Standard Error	0.357033764
Observations	5

ANOVA

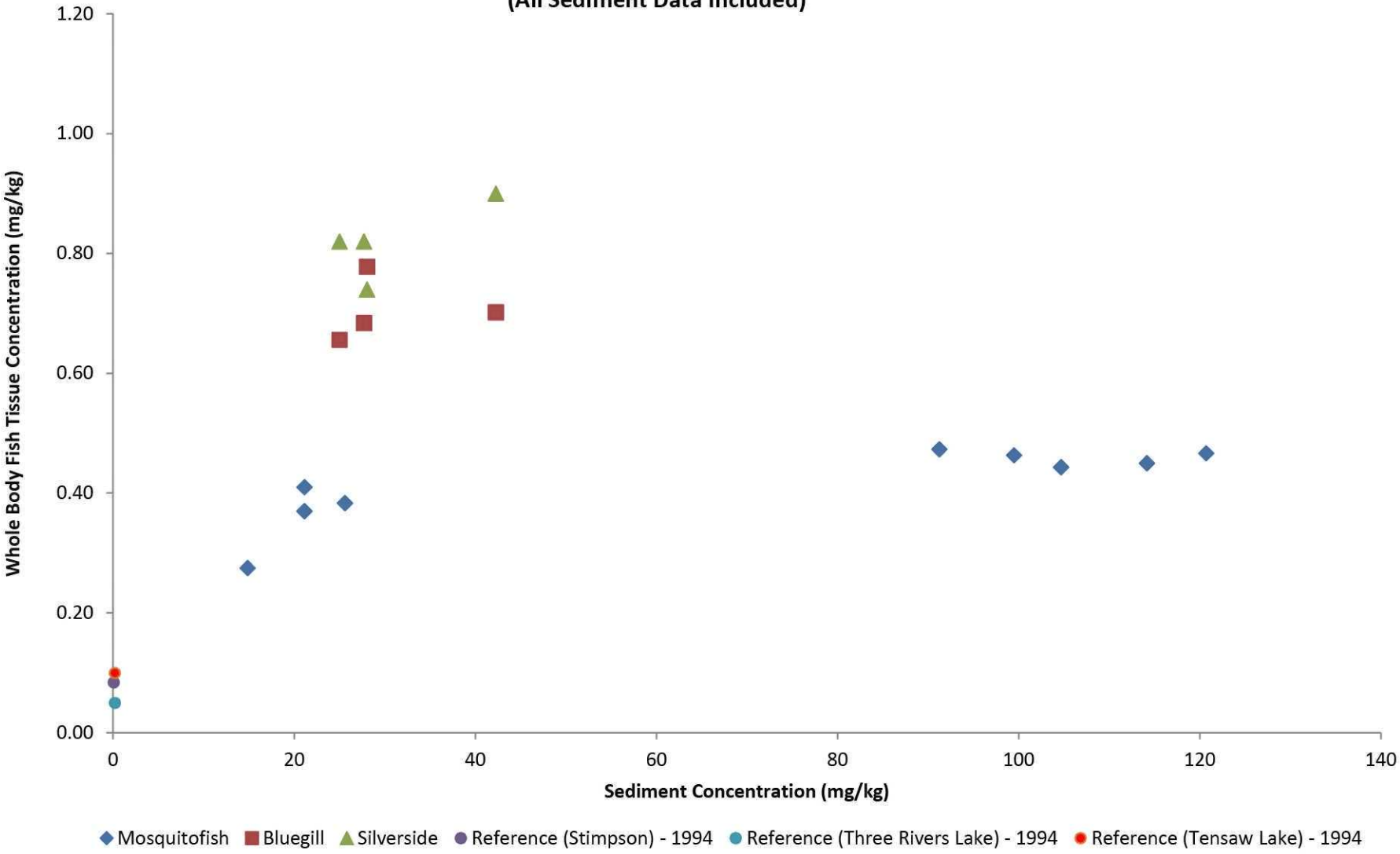
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.014150675	0.014150675	0.111009	0.760924998
Residual	3	0.382419325	0.127473108		
Total	4	0.39657			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	1.22004263	0.889478248	1.371638522	0.263758	-1.610674135	4.050759394	-1.610674135	4.050759394
X Variable 1	-0.003527598	0.010587657	-0.33318028	0.760925	-0.037222247	0.03016705	-0.037222247	0.03016705

FIGURE A-2a

Mercury in Forage Fish

Average Sediment Concentrations vs. Average Fish Concentrations
(All Sediment Data Included)



mg/kg = milligrams per kilogram

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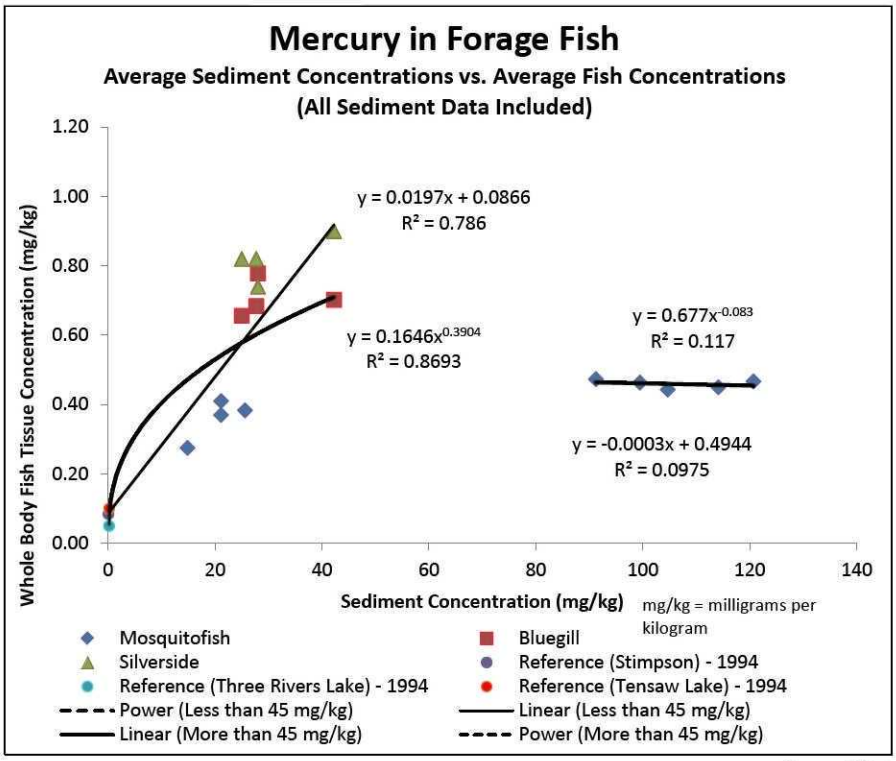
FIGURE A-2b



Prepared/Date: LSV 1/27/12
Checked/Date: MKB 1/30/12

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.312304
R Square	0.0975338
Adjusted R Square	-0.2032883
Standard Error	0.0135339
Observations	5

ANOVA

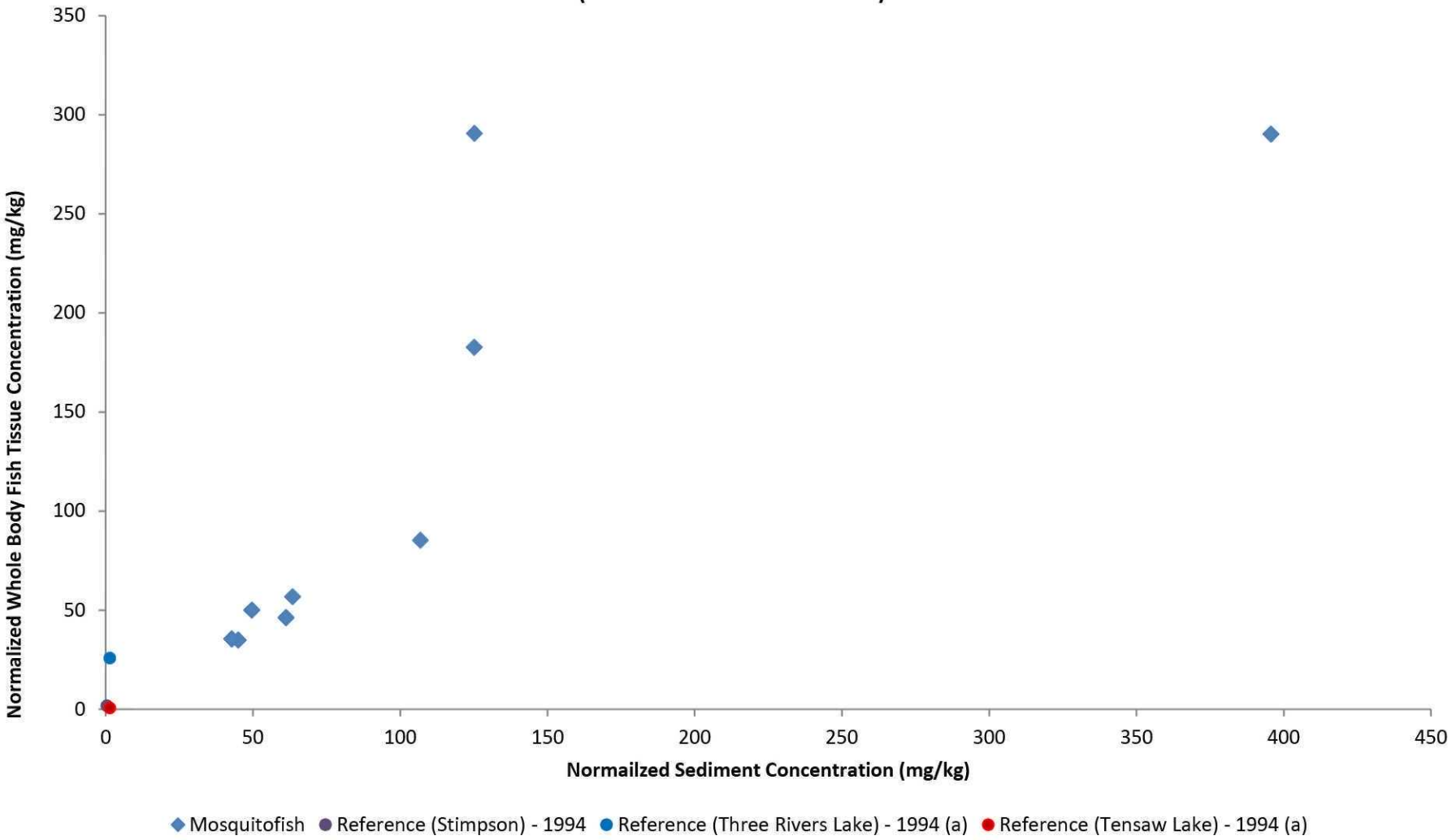
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.93872E-05	5.94E-05	0.324224	0.608924072
Residual	3	0.000549502	0.000183		
Total	4	0.000608889			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.4943507	0.061795116	7.999835	0.004077	0.297691074	0.69101035	0.297691074	0.69101035
X Variable 1	-0.0003302	0.00057996	-0.56941	0.608924	-0.002175925	0.00151546	-0.002175925	0.00151546

FIGURE A-3a

DDTR in Forage Fish

Average Normalized Sediment Concentrations vs. Average Normalized Fish Concentrations
(All Sediment Data Included)



mg/kg = milligrams per kilogram
(a) Sediment and fish concentrations are the calculated DDTR concentrations; only the 4,4-DDT, DDE, and DDD isomers data are available. The 4,4-isomer data were multiplied by 1.97 (a factor based on the sediment ratio of 2,4 to 4,4 DDT, DDE and DDD isomers) to generate the DDTR value for each sample.

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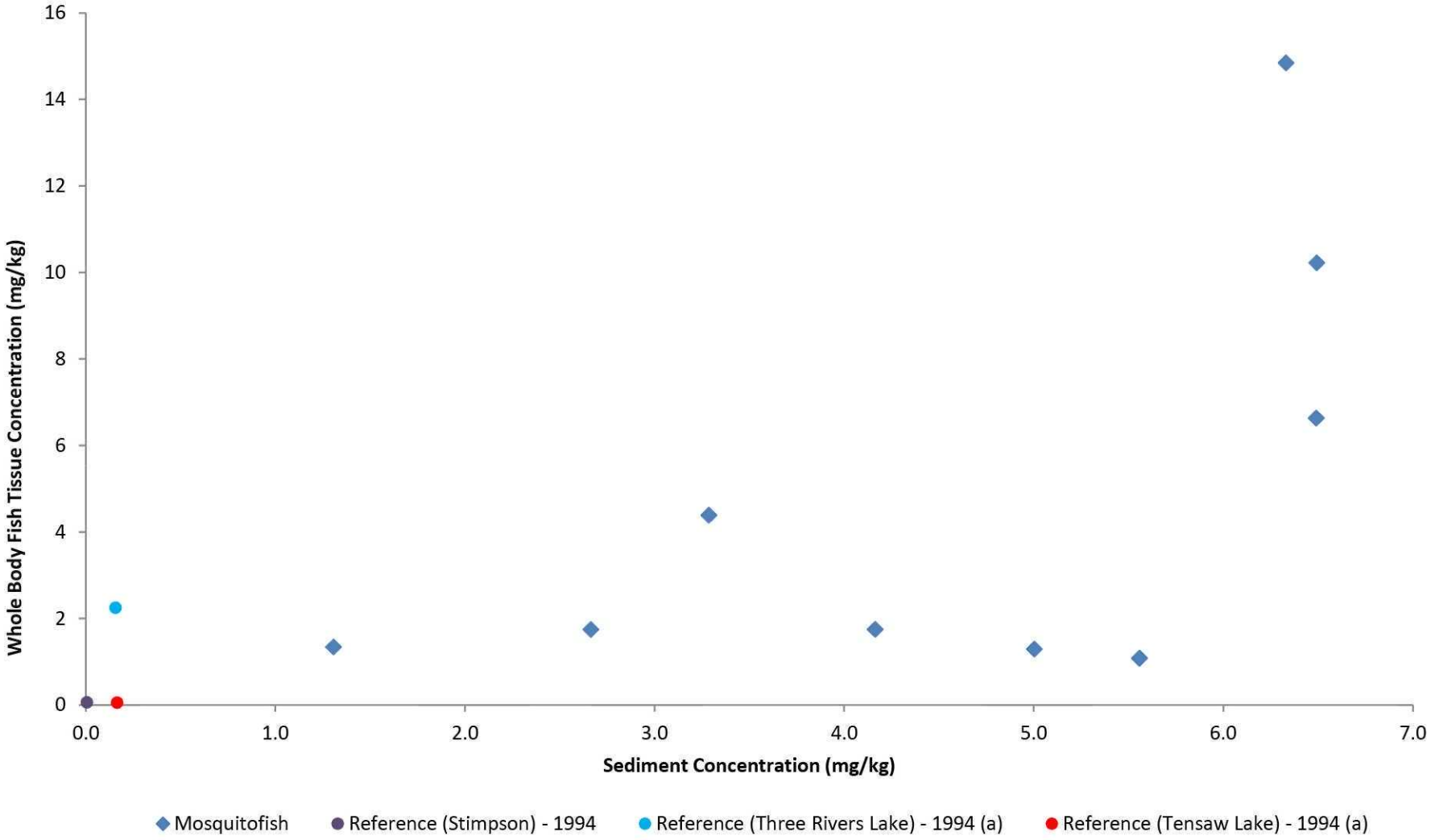
FIGURE A-3b

DDTR in Forage Fish

Average Sediment Concentrations vs. Average Fish Concentrations
(All Sediment Data Included)



mg/kg = milligrams per kilogram

(a) Sediment and fish concentrations are the calculated DDTR concentrations; only the 4,4-DDT, DDE, and DDD isomers data are available. The 4,4-isomer data were multiplied by 1.97 (a factor based on the sediment ratio of 2,4 to 4,4 DDT, DDE and DDD isomers) to generate the DDTR value for each sample.

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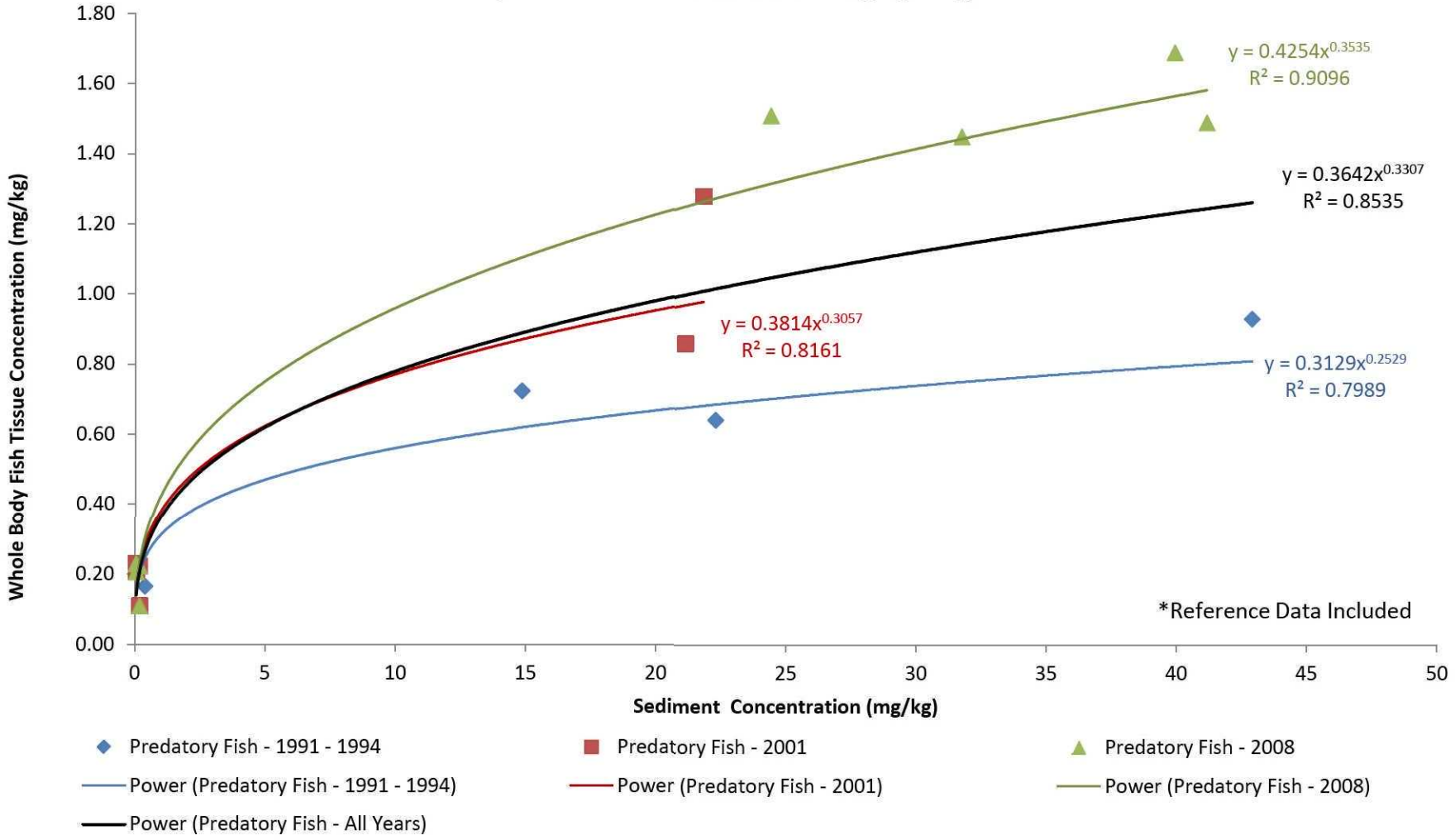
FIGURE A-4a

Mercury in Predatory Fish - Power Regression

Average Sediment Concentrations vs. Average Fish Concentrations
(Sediment Concentrations < 45 mg/kg Only)[a]



mg/kg = milligrams per kilogram
(a) Sediments greater than 45 mg/kg were excluded in PRG development because they are outside the observed range of bioaccumulation.

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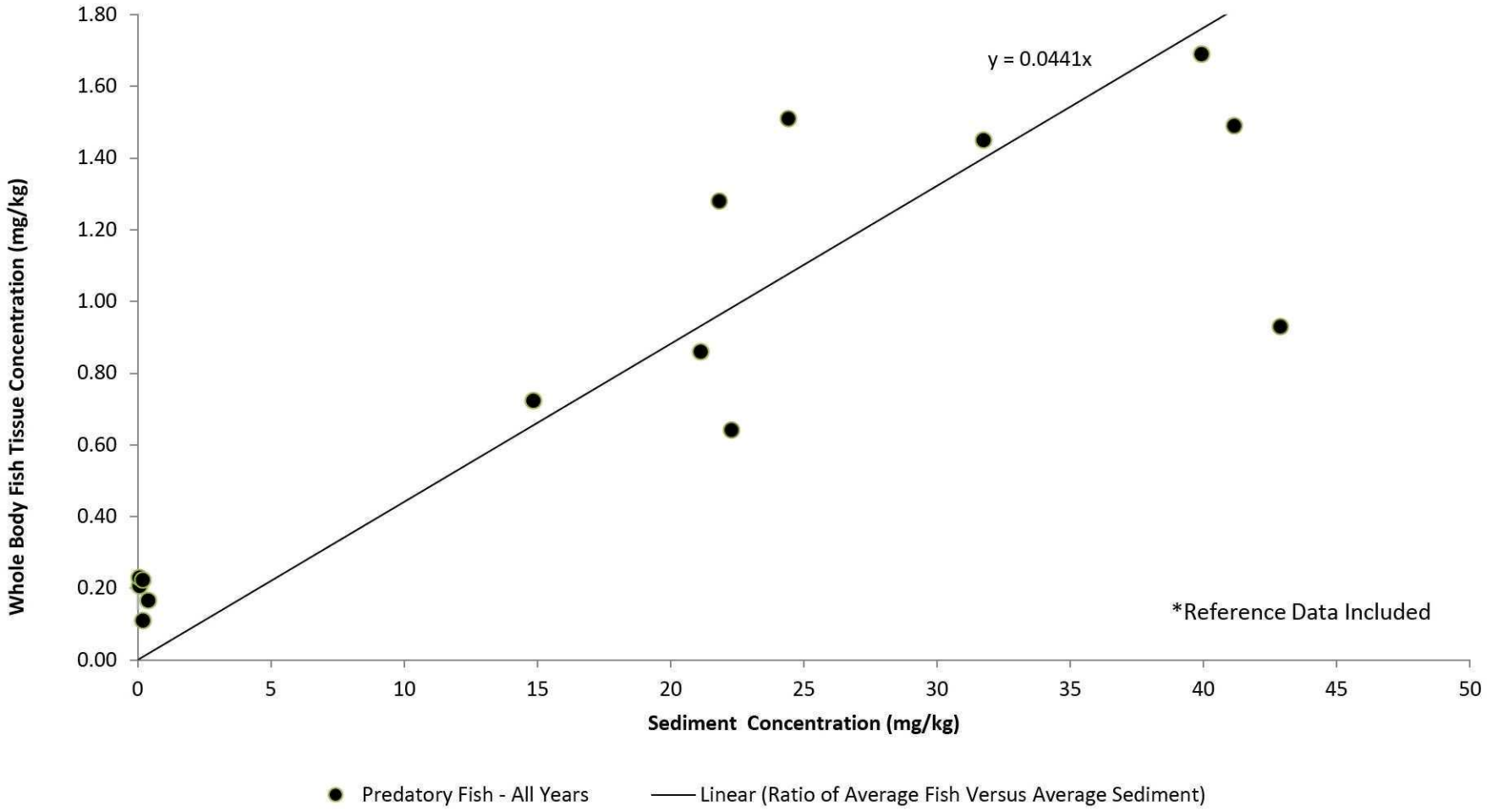
CHECKED BY/DATE: MKB 12/20/11

FIGURE A-4b

Mercury in Predatory Fish - Ratio Method for All Years

Average Sediment Concentrations vs. Average Fish Concentrations
(Sediment Concentrations < 45 mg/kg Only)[(a)]



mg/kg = milligrams per kilogram

(a) Sediments greater than 45 mg/kg were excluded in PRG development because they are outside the observed range of bioaccumulation.

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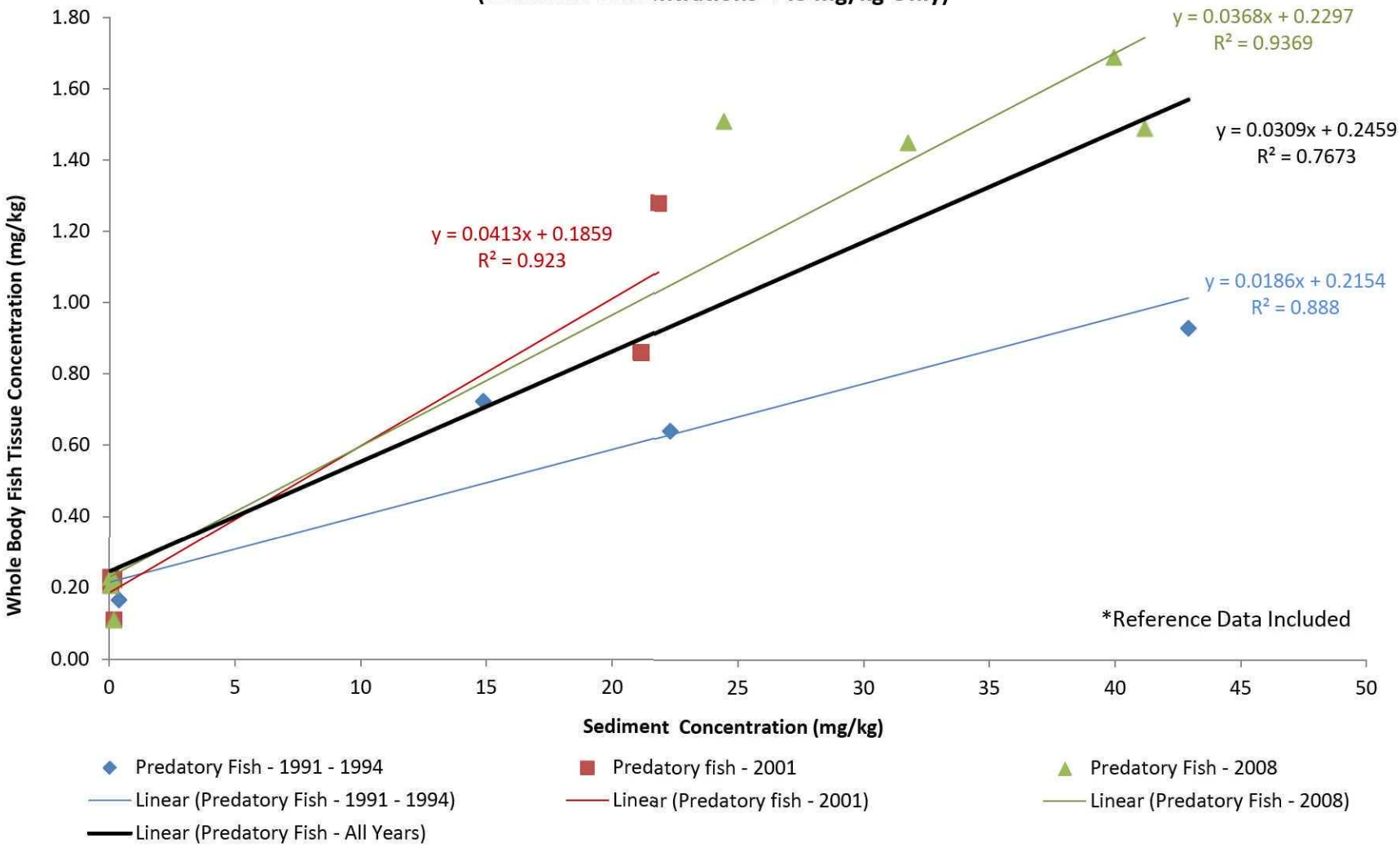
CHECKED BY/DATE:MKB 12/20/11

FIGURE A-4c

Mercury in Predatory Fish - Linear Regression

Average Sediment Concentrations vs. Average Fish Concentrations (Sediment Concentrations < 45 mg/kg Only)[a]

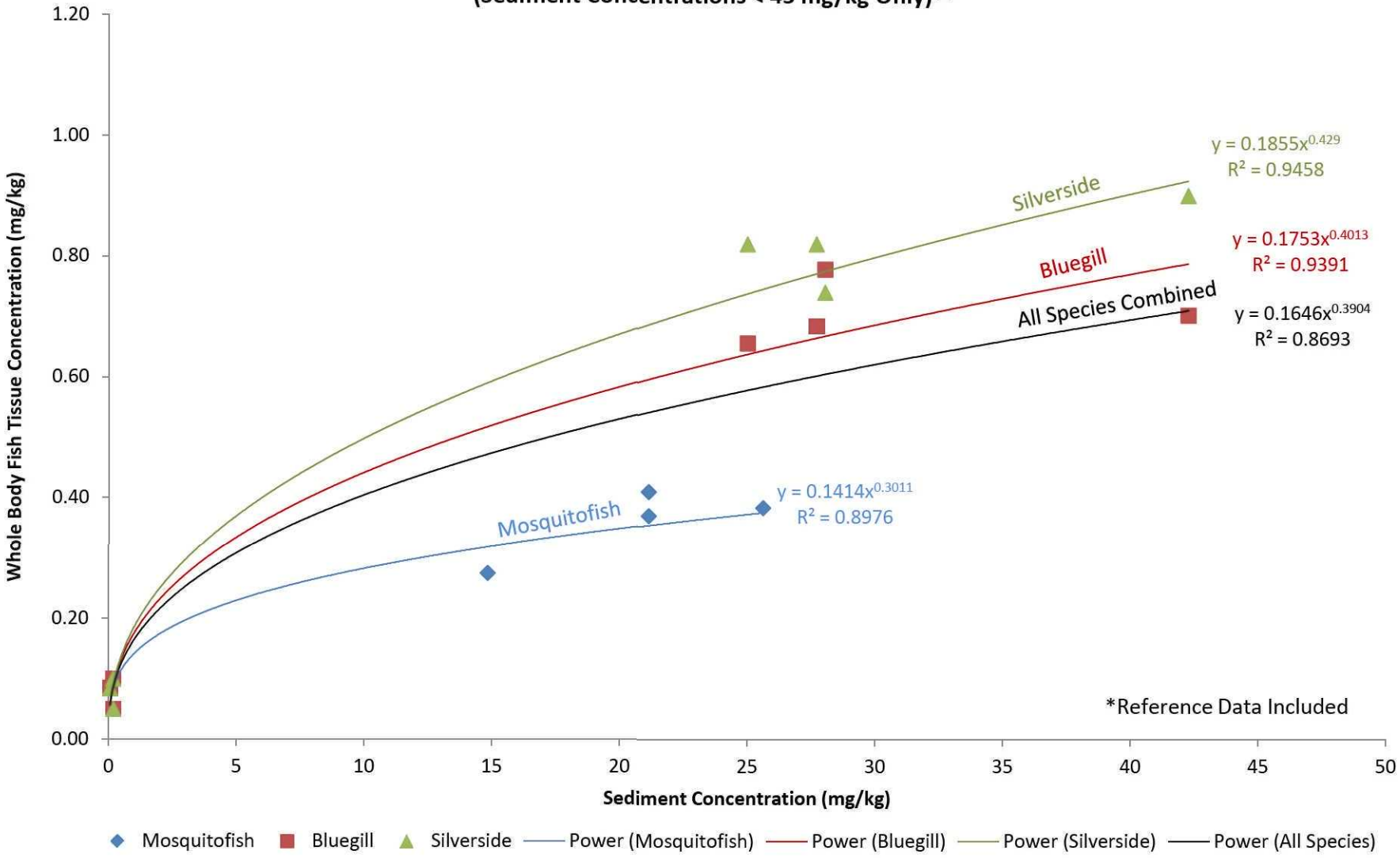


mg/kg = milligrams per kilogram

(a) Sediments greater than 45 mg/kg were excluded in PRG development because they are outside the observed range of bioaccumulation.

REVISED BY/DATE: NSR 12/19/11
CHECKED BY/DATE:MKB 12/20/11

FIGURE A-5a
Mercury in Forage Fish - Power Regression Analysis
Average Sediment Concentrations vs. Average Fish Concentrations
(Sediment Concentrations < 45 mg/kg Only)[a]



mg/kg = milligrams per kilogram

(a) Sediments greater than 45 mg/kg were excluded in PRG development because they are outside the observed range of bioaccumulation.

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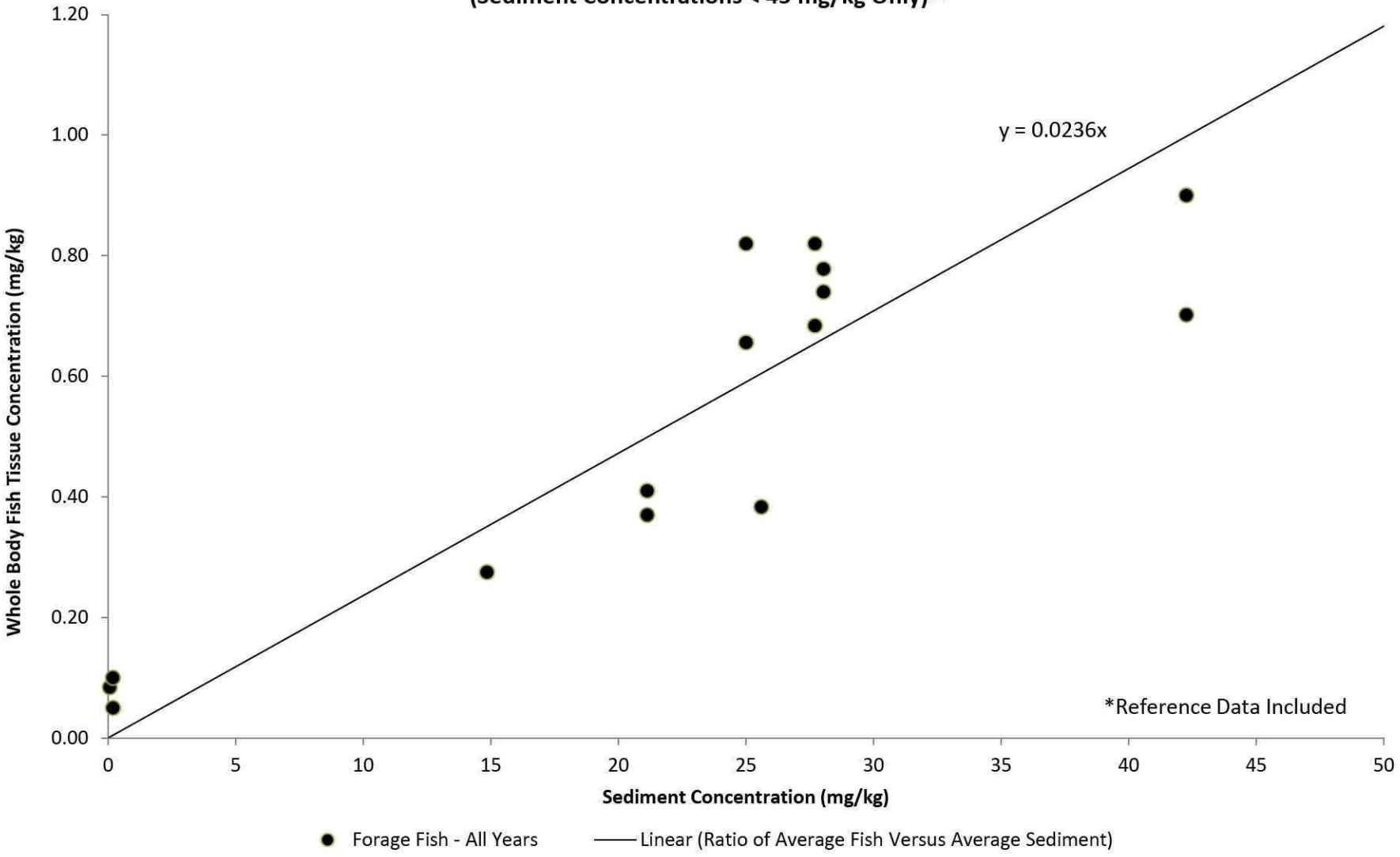
CHECKED BY/DATE: MKB 1/05/12

FIGURE A-5b
Mercury in Forage Fish - Ratio Method for All Years

Average Sediment Concentrations vs. Average Fish Concentrations
(Sediment Concentrations < 45 mg/kg Only)[a]



mg/kg = milligrams per kilogram

(a) Sediments greater than 45 mg/kg were excluded in PRG development because they are outside the observed range of bioaccumulation.

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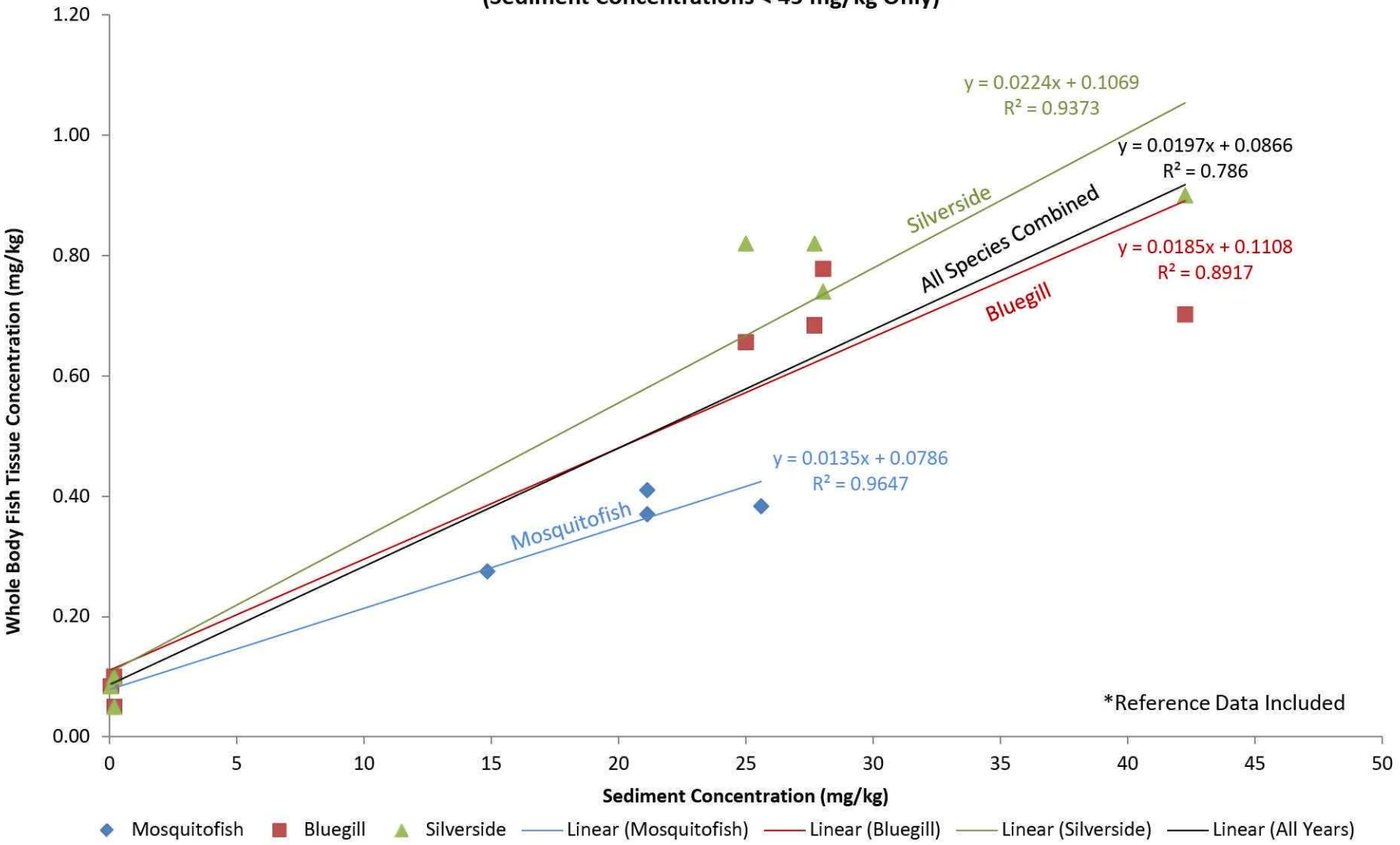
CHECKED BY/DATE: MKB 1/05/12

FIGURE A-5c
Mercury in Forage Fish - Linear Regression Analysis
Average Sediment Concentrations vs. Average Fish Concentrations
(Sediment Concentrations < 45 mg/kg Only)[a]



mg/kg = milligrams per kilogram

(a) Sediments greater than 45 mg/kg were excluded in PRG development because they are outside the observed range of bioaccumulation.

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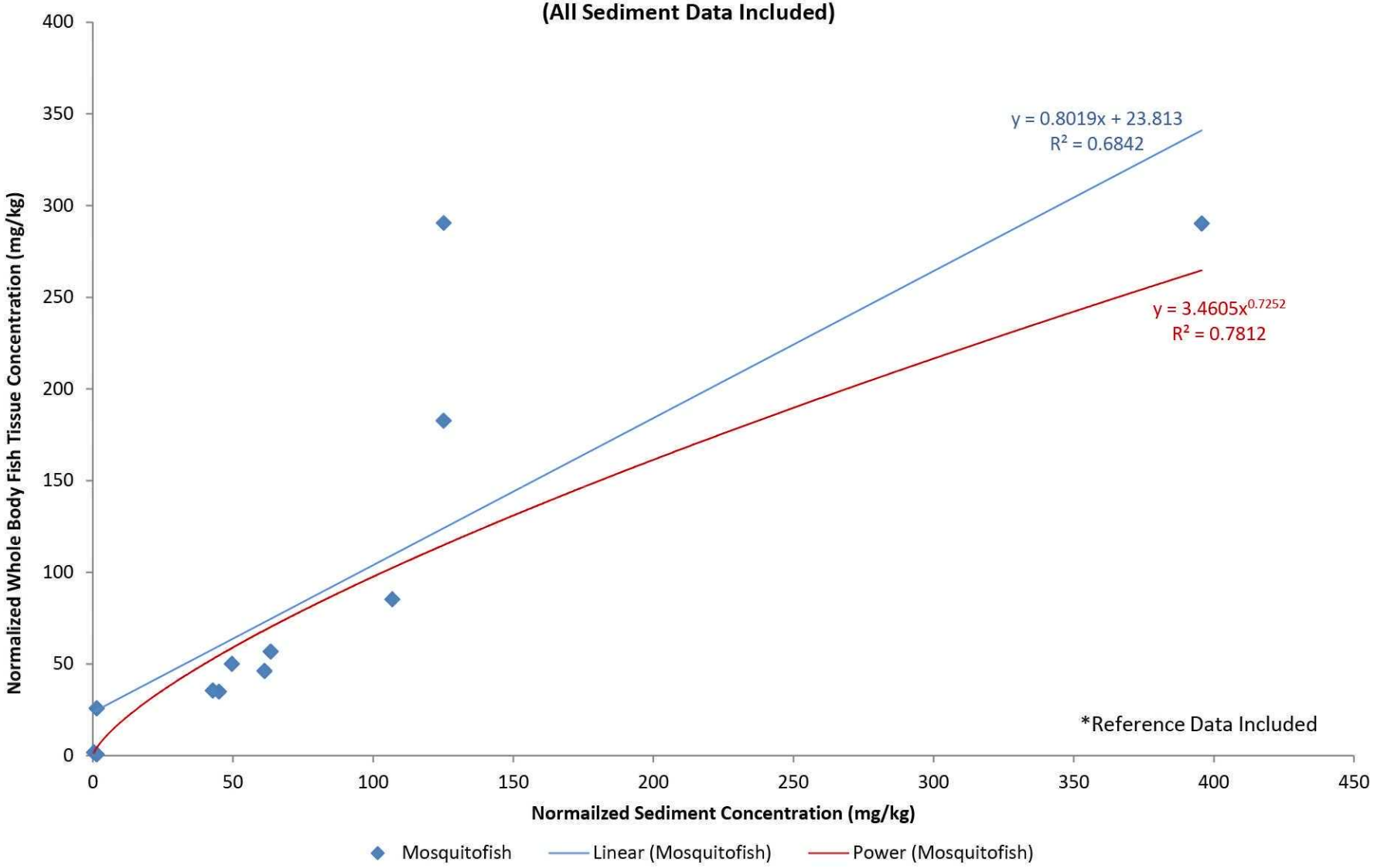
FIGURE A-6a

DDTR in Forage Fish

Average Normalized Sediment Concentrations vs. Average Normalized Fish Concentrations
(All Sediment Data Included)



mg/kg = milligrams per kilogram

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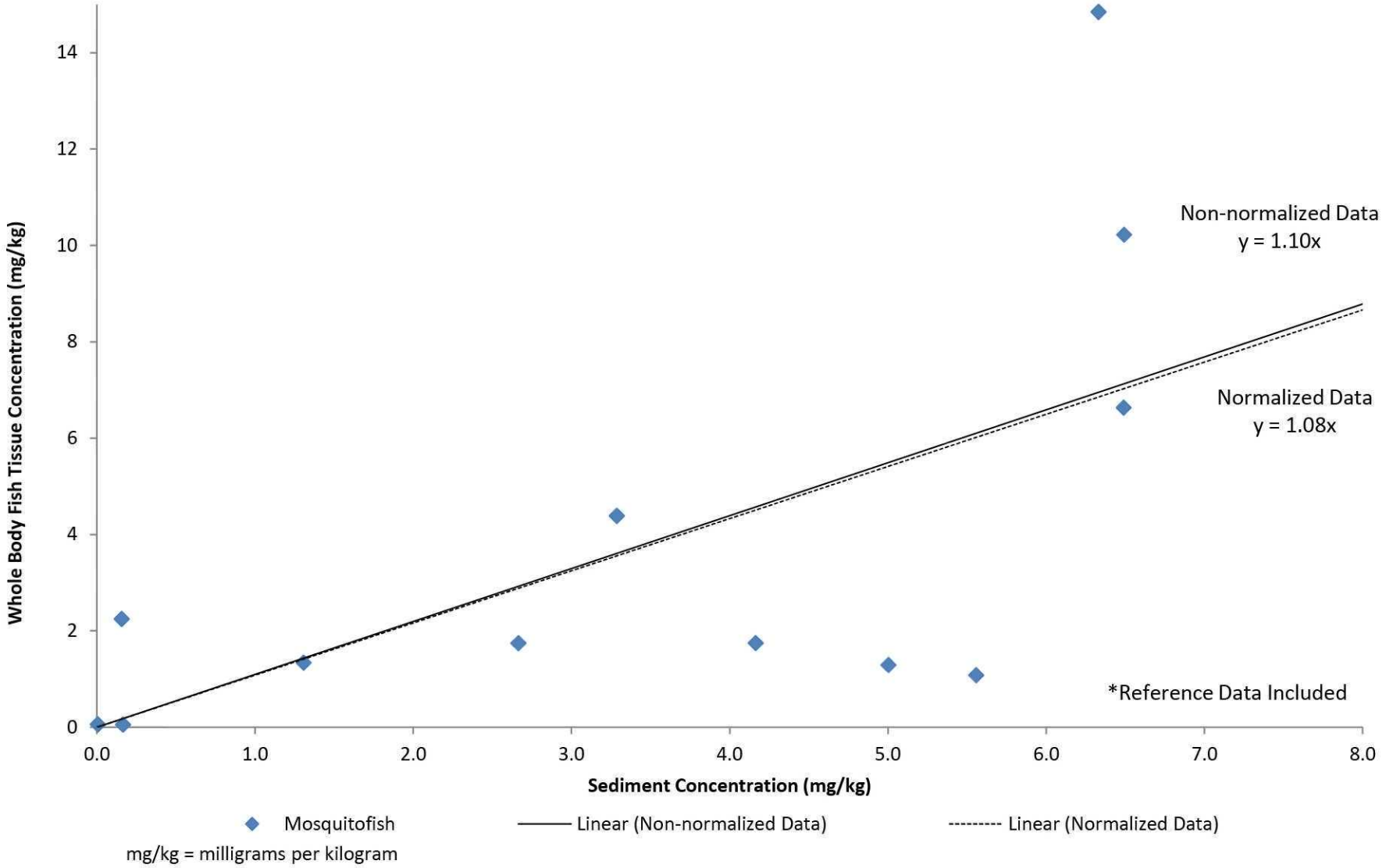
FIGURE A-6b

DDTR in Forage Fish - Ratio Method for All Years

Average Sediment Concentrations vs. Average Fish Concentrations
(All Sediment Data Included)



mg/kg = milligrams per kilogram

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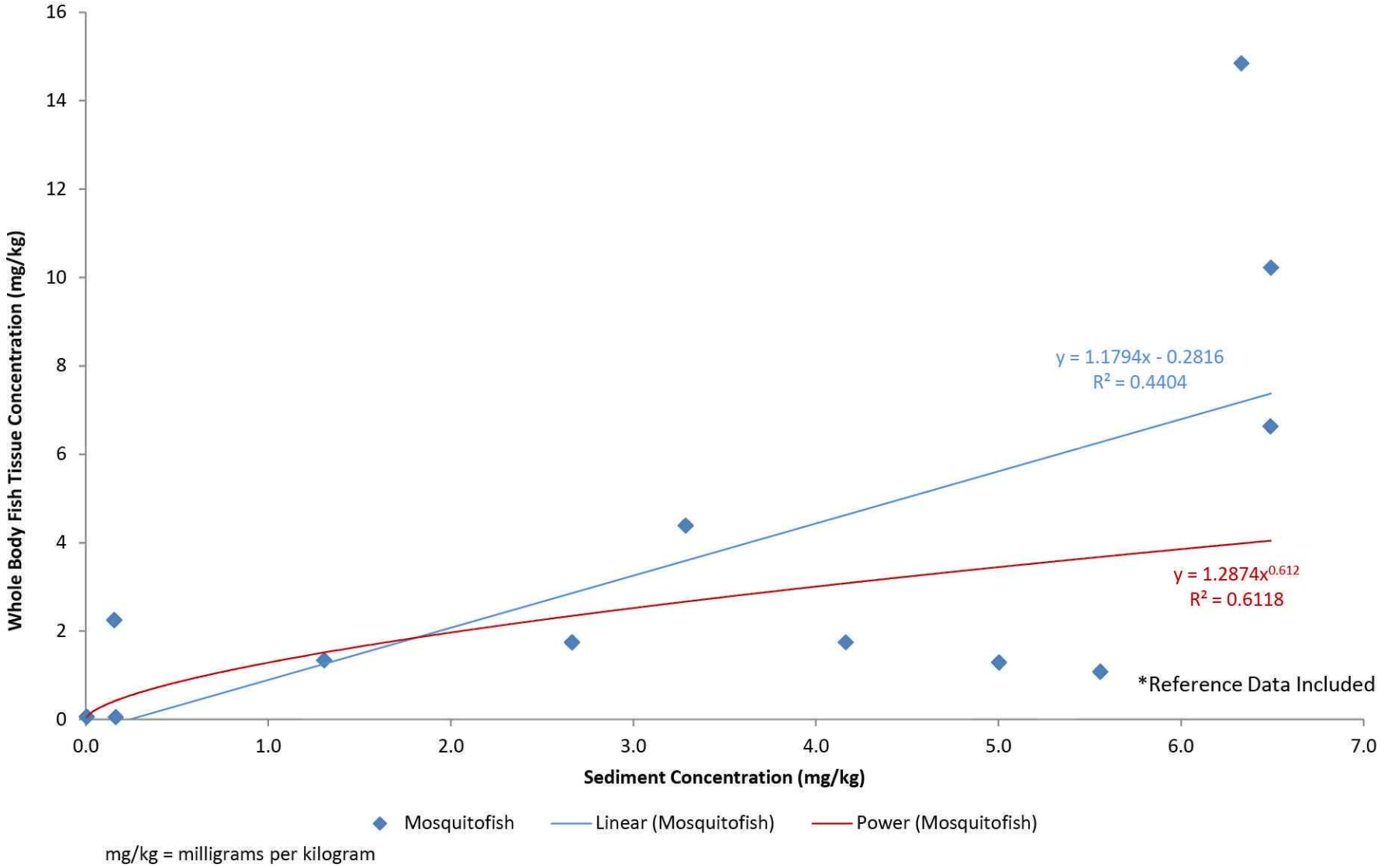
FIGURE A-6c

DDTR in Forage Fish

Average Sediment Concentrations vs. Average Fish Concentrations
(All Sediment Data Included)



mg/kg = milligrams per kilogram

PREPARED BY/DATE: NSR 12/21/11
CHECKED BY/DATE: MKB 1/05/12

APPENDIX A-2

Comparability of Statistical Parameters

APPENDIX A-2

COMPARABILITY OF STATISTICAL PARAMETERS

Least-Squares Linear Regression – p and R^2 Values

When interpreting the results of a least-squares linear regression (LSLR), two parameters are evaluated to determine whether a linear relationship is present between two variables: the p-value and the coefficient of determination (R^2). The p-value is the statistical probability of obtaining by chance a result at least as extreme as that observed. The coefficient of determination (R^2) is a measure of how accurate the regression model is of predicting the variable of interest. The p-value and R^2 value are key indicators of regression model quality. The p-value represents the statistical significance of a regression model, and the R^2 value represents the goodness of fit, or how well the regression line approximates the real data points.

The p-value is the probability that no relationship is present between the independent variable (plotted on the x-axis) and the dependent (or predicted) variable (plotted on the y-axis). A low probability (generally $p < 0.05$) indicates there is evidence (at a 95% confidence level) that a linear relationship is present between the two variables, and the results of the LSLR are statistically significant and meaningful. The lower the p-value, the higher the confidence is in the linear relationship. A p-value greater than 0.05 indicates a low confidence in the linear relationship described by the LSLR (Triola, 1986).

The measure of the relationship's strength is evaluated next if a significant relationship exists (based on the p-value). The R^2 value is a measure of how accurate the regression model is of predicting the dependent variable from the independent variable (Triola, 1986). The R^2 can vary between 0 (no predictive ability) and 1 (perfect prediction ability in that the regression line perfectly fits the data). An R^2 value greater ≥ 0.7 has been set as USEPA's goal for the McIntosh site. R^2 is determined as follows:

$$R^2 = \frac{explained\ variance}{total\ variance} = \frac{\Sigma(y' - \bar{y})^2}{\Sigma(y - \bar{y})^2} \quad \text{(Equation 1)}$$

Where:

y'	=	individual predicted data value
$\bar{y}$	=	mean value of all y data
y	=	individual data values

If each y estimate and the respective y values all are equal, the top and bottom parts of the equation are equal because the linear regression line passes through the mean y value and R^2 must equal 1.

The regression slope is 0 when there is no predictive ability, and the intercept is the mean of the y values because the regression line must pass through this value. Every value of x predicts y to be equal to the mean y value, and the top of Equation 1 becomes 0, resulting in an R^2 of 0 (Triola, 1986).

R^2 and p Values for Other Prediction Methods (Ratio Method)

R^2 and p-values have well defined meanings in LSLR, but neither are well defined with other methods of predictions, such as arithmetically-derived ratios (i.e., the ratio method). The descriptive equation for the ratio method is as follows:

$$y' = mx \quad \text{(Equation 2)}$$

Where:

m = slope (equivalent to ratio of average y-value to average x-value)

The R^2 value, as calculated for LSLR, has complications in interpretation using methods other than regression. Because Equation 2 is not required to pass through the mean y value, the "band" of variation in the estimated values may be shifted above or below the actual data set. The value of $\Sigma(y' - \bar{y})^2$ is no longer constrained by $\Sigma(y - \bar{y})^2$, and the R^2 can be values outside the range of 0 to 1 (Eisenhauer, 2003). An R^2 of 0.7 for the ratio method is no longer meaningful unless the range of possible R^2 values is known.

The value of m (slope) is defined outside of the regression process (by the experimental data) in the ratio method and is instead calculated to an exact non-zero defined value. A fixed positive defined slope would always have a p-value of zero. Therefore, unlike the p-value obtained using LSLR, analyzing a p-value is not a useful measurement for assessing the significance of the relationship described by Equation 2 (i.e., the ratio method).

R^2 and p-values that would be directly comparable to the R^2 and p-values generated from the linear and power regression models cannot be generated for the ratio method using the existing McIntosh datasets.

Citations

Triola, 1986. Elementary Statistics, 3rd Edition. The Benjamin/Cummings Publishing Company, Menlo Park, CA. ISBN 0-8053-9327-7

Eisenhauer, 2003. "Regression through the Origin"*Joseph G. Eisenhauer,* Canisius College, Buffalo, USA. *Teaching Statistics*. 25 (3): 76-80.
http://web.ist.utl.pt/~ist11038/compute/errtheory/,regression/regrthroughorigin.pdf

Additional Background Documents

University of Leicester, Online Statistics:
http://www.le.ac.uk/bl/gat/virtualfc/Stats/regression/regr1.html

Colby College, Regression Web page:
http://www.colby.edu/biology/BI17x/regression.html

APPENDIX A-3

Aquatic Data Pairings Regression Statistics – Fish Tissue and Sediment

Statistical Analysis of Mercury in Sediments and Predatory Fish

APPENDIX A-3
Statistical Analysis of Mercury in Sediments and Predatory Fish
1991 - 1994 Data Pairings
OLIN McINTOSH OU-2

Mercury In Predatory Fish, 1991 - 1994

Parameter	Location	Avg. Sed Conc. (mg/kg)	Log Avg. Sed. Conc. (mg/kg)	Avg. Fish Conc. (mg/kg)	Log Avg. Fish Conc. (mg/kg)
Largemouth Bass, WB	NW Basin	22	1.3	0.64	-0.2
Largemouth Bass, WB	SW Basin	42.9	1.6	0.93	0.0
Largemouth Bass, WB	Round Pond	15	1.2	0.72	-0.1
Largemouth Bass, WB	Reference Area - Stimpson	0.063	-1.2	0.21	-0.7
Largemouth Bass, WB	Reference Area - Ciba	0.057	-1.2	0.23	-0.6
Largemouth Bass, WB	Tombigbee River	0.39	-0.4	0.17	-0.8
Largemouth Bass, WB	Three Rivers Lake	0.19	-0.7	0.11	-1.0
Largemouth Bass, WB	Tensaw Lake	0.19	-0.7	0.22	-0.7

* Data pairs associated with sediment greater than 45 ppm excluded from anlaysis.

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.942352859
R Square	0.888028911
Adjusted R Square	0.869367063
Standard Error	5.695134436
Observations	8

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1543.406812	1543.406812	47.58526062	0.000458463
Residual	6	194.6073375	32.43455624		
Total	7	1738.014149			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-9.12871432	3.440041303	-2.653664162	0.037842892	-17.5461921	-0.711236505	-17.54619214	-0.711236505
X Variable 1	47.64297872	6.906574174	6.898207059	0.000458463	30.74320055	64.54275688	30.74320055	64.54275688

SUMMARY OUTPUT - POWER REGRESSION (USING LOG TRANSFORMED VALUES)

Regression Statistics	
Multiple R	0.893816464
R Square	0.79890787
Adjusted R Square	0.765392516
Standard Error	0.581132945
Observations	8

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	8.050148098	8.050148098	23.83707027	0.002759737
Residual	6	2.026292999	0.3377155		
Total	7	10.0764411			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	1.589807938	0.388516431	4.091996659	0.006414841	0.63914248	2.540473395	0.63914248	2.540473395
X Variable 1	3.158566565	0.646939391	4.882322221	0.002759737	1.575562905	4.741570226	1.575562905	4.741570226

APPENDIX A-3
Statistical Analysis of Mercury in Sediments and Predatory Fish
2001 Data Pairings
OLIN McINTOSH OU-2

Mercury In Predatory Fish, 2001

Parameter	Location	Avg. Sed Conc. (mg/kg)	Log Avg. Sed. Conc. (mg/kg)	Avg. Fish Conc. (mg/kg)	Log Avg. Fish Conc. (mg/kg)
Largemouth Bass, WB	SE Basin	22	1.3	1.28	0.1
Largemouth Bass, WB	Round Pond	21.1	1.3	0.86	-0.1
Largemouth Bass, WB	Reference Area-Stimpson	0.063	-1.2	0.21	-0.7
Largemouth Bass, WB	Reference Area-Ciba	0.057	-1.2	0.23	-0.6
Largemouth Bass, WB	Three Rivers Lake	0.19	-0.7	0.11	-1.0
Largemouth Bass, WB	Tensaw Lake	0.19	-0.7	0.22	-0.7

* Data pairs associated with sediment greater than 45 ppm excluded from anlaysis.

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.960754452
R Square	0.923049117
Adjusted R Square	0.903811396
Standard Error	3.420088098
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	561.236336	561.2363357	47.98121	0.002280096
Residual	4	46.7880104	11.6970026		
Total	5	608.024346			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-3.596148207	2.09687135	-1.7150066	0.161491	-9.417996404	2.22569999	-9.4179964	2.225699991
X Variable 1	22.34310818	3.22558129	6.926847031	0.00228	13.3874588	31.2987576	13.3874588	31.29875756

SUMMARY OUTPUT - POWER REGRESSION (USING LOG TRANSFORMED VALUES)

Regression Statistics	
Multiple R	0.903385147
R Square	0.816104724
Adjusted R Square	0.770130905
Standard Error	0.581298594
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.99837834	5.998378339	17.75151	0.013550722
Residual	4	1.35163222	0.337908056		
Total	5	7.35001056			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	1.079440454	0.38664915	2.791782827	0.049222	0.005930317	2.15295059	0.00593032	2.152950591
X Variable 1	2.669248949	0.63353619	4.213254126	0.013551	0.910270507	4.42822739	0.91027051	4.428227391

APPENDIX A-3
Statistical Analysis of Mercury in Sediments and Predatory Fish
2008 Data Pairings
OLIN McINTOSH OU-2

Mercury In Predatory Fish, 2008

Parameter	Location	Avg. Sed Conc. (mg/kg)	Log Avg. Sed. Conc. (mg/kg)	Avg. Fish Conc. (mg/kg)	Log Avg. Fish Conc. (mg/kg)
Largemouth Bass, WB	NE Basin	41	1.6	1.49	0.2
Largemouth Bass, WB	NW Basin	24.4	1.4	1.51	0.2
Largemouth Bass, WB	SE Basin	32	1.5	1.45	0.2
Largemouth Bass, WB	SW Basin	39.924	1.6	1.69	0.2
Largemouth Bass, WB	Reference Area - Stimpson	0.063	-1.2	0.21	-0.7
Largemouth Bass, WB	Reference Area - Ciba	0.057	-1.2	0.23	-0.6
Largemouth Bass, WB	Three Rivers Lake	0.19	-0.7	0.11	-1.0
Largemouth Bass, WB	Tensaw Lake	0.19	-0.7	0.22	-0.7

* Data pairs associated with sediment greater than 45 ppm excluded from anlaysis.

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.967985286
R Square	0.936995514
Adjusted R Square	0.926494766
Standard Error	5.144049741
Observations	8

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2361.171911	2361.17191	89.2313142	8.0076E-05
Residual	6	158.7674865	26.4612477		
Total	7	2519.939397			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-4.73606567	2.950924983	-1.60494275	0.15962869	-11.95671897	2.48458763	-11.95671897	2.484587629
X Variable 1	25.42665149	2.691723994	9.4462328	8.0076E-05	18.84024016	32.0130628	18.84024016	32.01306282

SUMMARY OUTPUT - POWER REGRESSION (USING LOG TRANSFORMED VALUES)

Regression Statistics	
Multiple R	0.953794362
R Square	0.909723686
Adjusted R Square	0.894677633
Standard Error	0.438910388
Observations	8

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	11.6476591	11.6476591	60.4626158	0.000238151
Residual	6	1.155853972	0.19264233		
Total	7	12.80351308			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.981116227	0.179786756	5.45711067	0.00157684	0.541193883	1.42103857	0.541193883	1.421038572
X Variable 1	2.569767427	0.330483936	7.77577107	0.00023815	1.76110237	3.37843248	1.76110237	3.378432484

APPENDIX A-3
Statistical Analysis of Mercury in Sediments and Predatory Fish
Data Pairings - All Years (1991 - 2008)
OLIN McINTOSH OU-2

Mercury In Predatory Fish, All Years

Parameter	Year	Location	Avg. Sed Conc. (mg/kg)	Log Avg. Sed. Conc. (mg/kg)	Avg. Fish Conc. (mg/kg)	Log Avg. Fish Conc. (mg/kg)
Largemouth Bass, WB	1994	NW Basin	22	1.3	0.64	-0.2
Largemouth Bass, WB	1994	SW Basin	42.9	1.6	0.93	0.0
Largemouth Bass, WB	1994	Round Pond	15	1.2	0.72	-0.1
Largemouth Bass, WB	1994	Reference Area - Stimpson	0.063	-1.2	0.21	-0.7
Largemouth Bass, WB	1991	Reference Area - Ciba	0.057	-1.2	0.23	-0.6
Largemouth Bass, WB	1992	Tombigbee River	0.39	-0.4	0.17	-0.8
Largemouth Bass, WB	1994	Three Rivers Lake	0.19	-0.7	0.11	-1.0
Largemouth Bass, WB	1994	Tensaw Lake	0.19	-0.7	0.22	-0.7
Largemouth Bass, WB	2001	SE Basin	22	1.3	1.28	0.1
Largemouth Bass, WB	2001	Round Pond	21.1	1.3	0.86	-0.1
Largemouth Bass, WB	2008	NE Basin	41	1.6	1.49	0.2
Largemouth Bass, WB	2008	NW Basin	24.4	1.4	1.51	0.2
Largemouth Bass, WB	2008	SE Basin	32	1.5	1.45	0.2
Largemouth Bass, WB	2008	SW Basin	39.924	1.6	1.69	0.2

* Data pairs associated with sediment greater than 45 ppm excluded from anlaysis.

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.875951
R Square	0.76729
Adjusted R Square	0.747897
Standard Error	8.239617
Observations	14

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2686.201468	2686.2015	39.56622	4.0061E-05
Residual	12	814.6954483	67.891287		
Total	13	3500.896917			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-1.76629	3.92200541	-0.450355	0.660483	-10.31161059	6.7790208	-10.31161059	6.779020804
X Variable 1	24.82888	3.947251765	6.2901684	4.01E-05	16.22855535	33.4292009	16.22855535	33.4292009

SUMMARY OUTPUT - POWER REGRESSION (USING LOG TRANSFORMED VALUES)

Regression Statistics	
Multiple R	0.923843
R Square	0.853486
Adjusted R Square	0.841277
Standard Error	0.464686
Observations	14

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	15.09445432	15.094454	69.90347	2.38668E-06
Residual	12	2.591193841	0.2159328		
Total	13	17.68564816			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	1.222212	0.14387867	8.4947378	2.02E-06	0.908726882	1.53569626	0.908726882	1.535696264
X Variable 1	2.581072	0.308710058	8.3608298	2.39E-06	1.908450803	3.25369367	1.908450803	3.25369367

Statistical Analysis of Mercury in Sediments and Forage Fish

APPENDIX A-3
Statistical Analysis of Mercury in Sediments and Forage Fish
All Species Combined
OLIN McINTOSH OU-2

Matrix	Area	Avg. Sediment Concentration (mg/kg)	Log Avg. Sediment Concentration (mg/kg)	Avg. Fish Tissue Concentration (mg/kg)	Log Avg. Fish Tissue Concentration (mg/kg)
Mosquitofish, WB - 1994	Reference-Stimpson	0.063	-1.203	0.084	-1.075
Forage Fish, WB	Reference-Tensaw Lake	0.19	-0.733	0.10	-1.000
Forage Fish, WB	Reference-Three Rivers	0.19	-0.721	0.05	-1.301
Mosquitofish, WB	Round Pound	15	1.172	0.275	-0.561
Mosquitofish, WB	Round Pound	21	1.325	0.41	-0.387
Mosquitofish, WB	Round Pound	21	1.325	0.37	-0.432
Silverside, Comp	SE Basin	25	1.398	0.82	-0.086
Bluegill, WB	SE Basin	25	1.398	0.66	-0.183
Mosquitofish, WB	SE Basin	26	1.408	0.38	-0.416
Silverside, Comp	NW Basin	28	1.442	0.82	-0.086
Bluegill, WB	NW Basin	28	1.442	0.684	-0.165
Silverside, Comp	SW Basin	28	1.448	0.74	-0.131
Bluegill, WB	SW Basin	28	1.448	0.78	-0.109
Silverside, Comp	NE Basin	42	1.626	0.9	-0.046
Bluegill, WB - 2008	NE Basin	42	1.626	0.702	-0.154

Notes:
* Data pairs associated with sediment greater than 45 ppm excluded from anlaysis.
(a) Sediment concentration is the average of the parent sample and the duplicate sample.
(b) Sediment concentration is the average of a 5-point composite sample.
WB = Whole Body
Comp = Composite Sample
NW = Northwest
NE = Northeast
SW = Southwest
SE = Southeast
NA = Not Applicable

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.886549985
R Square	0.785970875
Adjusted R Square	0.769507097
Standard Error	6.383141066
Observations	15

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1945.117384	1945.117384	47.73939717	1.07004E-05
Residual	13	529.6783683	40.74448987		
Total	14	2474.795753			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	1.237056137	3.419827006	0.361730618	0.723364953	-6.151030922	8.6251432	-6.15103092	8.625143196
X Variable 1	39.95590597	5.782857852	6.909370244	1.07004E-05	27.46280115	52.449011	27.46280115	52.44901079

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.932386748
R Square	0.869345047
Adjusted R Square	0.859294666
Standard Error	0.362768919
Observations	15

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	11.38334244	11.38334244	86.49871546	4.14558E-07
Residual	13	1.710816755	0.131601289		
Total	14	13.0941592			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	1.870221808	0.135466225	13.80581618	3.82441E-09	1.577564821	2.1628788	1.577564821	2.162878795
X Variable 1	2.226646362	0.239412278	9.300468561	4.14558E-07	1.709427582	2.7438651	1.709427582	2.743865142

APPENDIX A-3
Statistical Analysis of Mercury in Sediments and Forage Fish
Mosquitofish
OLIN McINTOSH OU-2

Matrix	Area	Avg. Sediment Concentration (mg/kg)	Log Avg. Sediment Concentration (mg/kg)	Avg. Fish Tissue Concentration (mg/kg)	Log Avg. Fish Tissue Concentration (mg/kg)
Mosquitofish, WB - 1994	Reference-Stimpson	0.063	-1.203	0.084	-1.075
Forage Fish, WB	Reference-Tensaw Lake	0.19	-0.733	0.10	-1.000
Forage Fish, WB	Reference-Three Rivers	0.19	-0.721	0.05	-1.301
Mosquitofish, WB	Round Pound	15	1.172	0.275	-0.561
Mosquitofish, WB	Round Pound	21	1.325	0.41	-0.387
Mosquitofish, WB	Round Pound	21	1.325	0.37	-0.432
Mosquitofish, WB	SE Basin	26	1.408	0.38	-0.416

Notes:
* Data pairs associated with sediment greater than 45 ppm excluded from anlaysis.
(a) Sediment concentration is the average of the parent sample and the duplicate sample.
(b) Sediment concentration is the average of a 5-point composite sample.
WB = Whole Body
Comp = Composite Sample
NW = Northwest
NE = Northeast
SW = Southwest
SE = Southeast
NA = Not Applicable

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.982181503
R Square	0.964680506
Adjusted R Square	0.957616607
Standard Error	2.348885599
Observations	7

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	753.4644418	753.4644418	136.5648811	8.06256E-05
Residual	5	27.58631779	5.517263558		
Total	6	781.0507596			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-5.197890908	1.709639464	-3.04034331	0.028739492	-9.592659059	-0.8031228	-9.59265906	-0.803122757
X Variable 1	71.46090139	6.115035386	11.68609777	8.06256E-05	55.7417025	87.1801003	55.7417025	87.18010027

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.947419343
R Square	0.897603411
Adjusted R Square	0.877124094
Standard Error	0.415376905
Observations	7

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	7.562296511	7.562296511	43.8297517	0.001183517
Residual	5	0.862689865	0.172537973		
Total	6	8.424986375			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.570295954	0.367910332	6.986202163	0.000925108	1.624552339	3.51603957	1.624552339	3.51603957
X Variable 1	2.981380074	0.450332032	6.620404195	0.001183517	1.823764733	4.13899541	1.823764733	4.138995415

APPENDIX A-3
Statistical Analysis of Mercury in Sediments and Forage Fish
Bluegill
OLIN McINTOSH OU-2

Matrix	Area	Avg. Sediment Concentration (mg/kg)	Log Avg. Sediment Concentration (mg/kg)	Avg. Fish Tissue Concentration (mg/kg)	Log Avg. Fish Tissue Concentration (mg/kg)
Mosquitofish, WB - 1994	Reference-Stimpson	0.063	-1.203	0.084	-1.075
Forage Fish, WB	Reference-Tensaw Lake	0.19	-0.733	0.10	-1.000
Forage Fish, WB	Reference-Three Rivers	0.19	-0.721	0.05	-1.301
Bluegill, WB	SE Basin	25	1.398	0.66	-0.183
Bluegill, WB	NW Basin	28	1.442	0.684	-0.165
Bluegill, WB	SW Basin	28	1.448	0.78	-0.109
Bluegill, WB	NE Basin	42	1.626	0.702	-0.154

Notes:
* Data pairs associated with sediment greater than 45 ppm excluded from anlaysis.
(a) Sediment concentration is the average of the parent sample and the duplicate sample.
(b) Sediment concentration is the average of a 5-point composite sample.
WB = Whole Body
Comp = Composite Sample
NW = Northwest
NE = Northeast
SW = Southwest
SE = Southeast
NA = Not Applicable

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.944299993
R Square	0.891702477
Adjusted R Square	0.870042973
Standard Error	6.222193982
Observations	7

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1593.890741	1593.890741	41.16910777	0.001364609
Residual	5	193.5784897	38.71569795		
Total	6	1787.469231			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-3.440051438	4.039417945	-0.851620576	0.433308638	-13.82370583	6.94360295	-13.8237058	6.943602954
X Variable 1	48.29730752	7.527264777	6.416315747	0.001364609	28.94785742	67.6467576	28.94785742	67.64675763

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.969095273
R Square	0.939145648
Adjusted R Square	0.926974778
Standard Error	0.344713404
Observations	7

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	9.169119934	9.169119934	77.16339232	0.000317167
Residual	5	0.594136653	0.118827331		
Total	6	9.763256588			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	1.798246869	0.200004507	8.991031725	0.000284022	1.284118916	2.31237482	1.284118916	2.312374822
X Variable 1	2.340524954	0.266445027	8.784269595	0.000317167	1.655606206	3.0254437	1.655606206	3.025443701

APPENDIX A-3
Statistical Analysis of Mercury in Sediments and Forage Fish
Silverside
OLIN McINTOSH OU-2

Matrix	Area	Avg. Sediment Concentration (mg/kg)	Log Avg. Sediment Concentration (mg/kg)	Avg. Fish Tissue Concentration (mg/kg)	Log Avg. Fish Tissue Concentration (mg/kg)
Mosquitofish, WB - 1994	Reference-Stimpson	0.063	-1.203	0.084	-1.075
Forage Fish, WB	Reference-Tensaw Lake	0.19	-0.733	0.10	-1.000
Forage Fish, WB	Reference-Three Rivers	0.19	-0.721	0.05	-1.301
Silverside, Comp	SE Basin	25	1.398	0.82	-0.086
Silverside, Comp	NW Basin	28	1.442	0.82	-0.086
Silverside, Comp	SW Basin	28	1.448	0.74	-0.131
Silverside, Comp	NE Basin	42	1.626	0.9	-0.046

Notes:
* Data pairs associated with sediment greater than 45 ppm excluded from anlaysis.
(a) Sediment concentration is the average of the parent sample and the duplicate sample.
(b) Sediment concentration is the average of a 5-point composite sample.
WB = Whole Body
Comp = Composite Sample
NW = Northwest
NE = Northeast
SW = Southwest
SE = Southeast
NA = Not Applicable

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.968158525
R Square	0.937330929
Adjusted R Square	0.924797115
Standard Error	4.73326601
Observations	7

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1675.450195	1675.450195	74.78417333	0.000341577
Residual	5	112.0190356	22.40380712		
Total	6	1787.469231			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-3.364378318	3.015920064	-1.115539619	0.315343541	-11.11704765	4.388291013	-11.1170476	4.388291013
X Variable 1	41.82451455	4.83644285	8.647784302	0.000341577	29.39204242	54.25698669	29.3920424	54.25698669

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.972537608
R Square	0.945829399
Adjusted R Square	0.934995279
Standard Error	0.325232678
Observations	7

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	9.234375113	9.234375113	87.30098846	0.000236527
Residual	5	0.528881475	0.105776295		
Total	6	9.763256588			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	1.638353349	0.175708902	9.324247811	0.000238864	1.186679236	2.090027461	1.18667924	2.090027461
X Variable 1	2.204558546	0.235945694	9.343499797	0.000236527	1.598040831	2.811076262	1.59804083	2.811076262

Statistical Analysis of DDTR in Sediments and Forage Fish

APPENDIX A-3
Statistical Analysis of DDTR in Sediments and Forage Fish
Normalized Data
OLIN McINTOSH OU-2

Matrix	Year	Area	Norm. Avg. Sed. Conc. (mg/kg)	Log Norm. Avg. Sed. Conc. (mg/kg)	Avg. Norm. Fish Tissue Concentration (mg DDTR/kg lipid)	Log Avg. Norm. Fish Tissue Concentration (mg DDTR/kg lipid)
Mosquitofish, WB	1991, 1994	NE Basin	107	2.03	85	1.93
Mosquitofish, WB	1994	Round Pond	396	2.60	290	2.46
Mosquitofish, WB	2001	NW Basin	63	1.80	57	1.75
Mosquitofish, WB	2001	NE Basin	50	1.70	50	1.70
Mosquitofish, WB	2001	NE Basin	45	1.65	35.0	1.54
Mosquitofish, WB	2001	NE Basin	43	1.63	36	1.55
Mosquitofish, WB	2001	SE Basin	61	1.79	46	1.67
Mosquitofish, WB	2001	Round Pond	125	2.10	291	2.46
Mosquitofish, WB	2001	Round Pond	125	2.10	183	2.26
Mosquitofish, WB	1994	Reference-Stimpson	0.33	-0.48	1.88	0.27
Forage Fish, WB	1994	Reference-Three Rivers	1.33	0.13	25.9	1.41
Forage Fish, WB	1994	Reference-Tensaw Lake	1.33	0.12	0.782	-0.11

Notes:
WB = Whole Body
NW = Northwest
NE = Northeast
SW = Southwest
SE = Southeast

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.827135653
R Square	0.684153388
Adjusted R Square	0.652568727
Standard Error	63.34170751
Observations	12

ANOVA

	df	*SS*	*F*
Regression	1	86907.40708	21.66093802
Residual	10	40121.7191	
Total	11	127029.1262	

	Coefficients	*Standard Error*	*P-value*	*Upper 95%*	*Lower 95.0%*
Intercept	6.464171896	24.85129606	0.800053057	61.83630992	-48.90796613
X Variable 1	0.853189995	0.18331885	0.000902345	1.261649845	0.444730145

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.883946099
R Square	0.781360706
Adjusted R Square	0.759496776
Standard Error	0.469351973
Observations	12

ANOVA

	df	*SS*	*F*
Regression	1	7.872644569	35.73743263
Residual	10	2.202912741	
Total	11	10.07555731	

	Coefficients	*Standard Error*	*P-value*	*Upper 95%*	*Lower 95.0%*
Intercept	-0.268321516	0.314771508	0.413923643	0.433033108	-0.969676141
X Variable 1	1.077435461	0.180231041	0.000136032	1.479015244	0.675855679

APPENDIX A-3
Statistical Analysis of DDTR in Sediments and Forage Fish
Non-Normalized Data
OLIN McINTOSH OU-2

Matrix	Year	Area	Avg. Sediment Concentration (mg/kg)	Log Avg. Sediment Concentration (mg/kg)	Avg. Fish Tissue Concentration (mg DDTR/kg lipid)	Log Avg. Fish Tissue Concentration (mg DDTR/kg lipid)
Mosquitofish, WB	1991, 1994	NE Basin	3.29	0.52	4.39	0.64
Mosquitofish, WB	1994	Round Pond	6.33	0.80	14.9	1.17
Mosquitofish, WB	2001	NW Basin	2.66	0.43	1.75	0.24
Mosquitofish, WB	2001	NE Basin	4.16	0.62	1.75	0.24
Mosquitofish, WB	2001	NE Basin	5.00	0.70	1.30	0.11
Mosquitofish, WB	2001	NE Basin	5.56	0.74	1.08	0.03
Mosquitofish, WB	2001	SE Basin	1.31	0.12	1.350	0.13
Mosquitofish, WB	2001	Round Pond	6.5	0.81	10.20	1.01
Mosquitofish, WB	2001	Round Pond	6.5	0.81	6.64	0.82

Notes:
(a) Sediment concentration is the average of the parent sample and the duplicate sample.
(b) Concentration is the calculated DDTR concentration; only the 4,4-DDT, DDE, and DDD isomers data are available. The used for the non-detect isomers.
WB = Whole Body
NW = Northwest
NE = Northeast
SW = Southwest
SE = Southeast

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.66345353
R Square	0.44017058
Adjusted R Square	0.38418764
Standard Error	2.02026677
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	32.09096267	32.09096267	7.862584085	0.018665063
Residual	10	40.81477835	4.081477835		
Total	11	72.90574102			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.04538846	0.77291533	2.646329267	0.024466726	0.32322579	3.767551128	0.32322579	3.767551128
X Variable 1	0.37361049	0.133240549	2.804029972	0.018665063	0.07673205	0.670488934	0.07673205	0.670488934

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.78264485
R Square	0.61253296
Adjusted R Square	0.57378626
Standard Error	0.63087781
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	6.291949086	6.291949086	15.80864685	0.002617792
Residual	10	3.980068089	0.398006809		
Total	11	10.27201718			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-0.0568825	0.188484676	-0.301788668	0.768995956	-0.476852568	0.363087489	-0.47685257	0.363087489
X Variable 1	1.00000821	0.251510555	3.97600891	0.002617792	0.43960777	1.560408643	0.43960777	1.560408643

APPENDIX B

Determination of Target Fish Tissue Concentration by Back Calculation of Risk Equations

TABLE B-1

TARGET MERCURY CONCENTRATION IN SEDIMENT - NOAEL RISK
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_{FF}	C_{FF}	P_{PF}	C_{PF}	P_{CR}	C_{CR}	P_{AM}	C_{AM}	P_{VP}	$C_{VP,T}$	$C_{VP,A}$	P_S	EDD [(a)] (mg/kg-day)	NOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Aquatic Receptors																							
Mink	Mercury	1.69E-04	2.0	27	0.852	0.134	0.710	1.00	0.05	0.048	0.20	0.095	0.10	0.077	0.25	0.193	0.40	0.259	0.316	0.09	3.69E-01	0.370	**1.0**

Notes:

PREPARED BY/DATE: MKB 5/17/11
CHECKED BY/DATE: NSR 5/20/11

(a) EDD (mg/kg·day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)] + (IRW x CW)/BW

Aquatic vertebrate prey items used for the mink.

Green highlighted entries represent target concentrations in controlling media needed to achieve the target HQ=1.

TABLE B-2

NOAEL RISK CALCULATIONS - METHYLMERCURY
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_{AI}	C_{AI}	P_{FF}	C_{FF}	P_{PF}	C_{PF}	P_{CR}	C_{CR}	P_{AM}	C_{AM}	P_S	EDD [(a)] (mg/kg-day)	NOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Aquatic Receptors																						
Pied-Billed Grebe	Methylmercury	2.74E-06	0.0051	0.00728	0.417	0.404	0.0328	1.00	0.60	0.019	0.20	0.58	0.00	1.495	0.20	0.107	0.00	0.104	0.03	6.02E-02	0.060	**1.0**
Belted Kingfisher (Maximum Exposure)	Methylmercury	2.74E-06	0.0051	0.00728	0.152	0.566	0.0170	1.00	0.00	0.019	1.00	0.11	0.00	1.495	0.00	0.107	0.00	0.104	0.00	6.00E-02	0.060	**1.0**
Belted Kingfisher (Central Tendency)	Methylmercury	2.74E-06	0.0051	0.00728	0.152	0.566	0.0170	0.50	0.19	0.019	0.51	0.35	0.00	1.495	0.05	0.107	0.25	0.104	0.00	5.98E-02	0.060	**1.0**
Little Blue Heron	Methylmercury	2.74E-06	0.0051	0.00728	0.340	0.432	0.160	0.90	0.25	0.019	0.75	0.20	0.00	1.495	0.00	0.107	0.00	0.104	0.03	6.03E-02	0.060	**1.0**
Great Blue Heron	Methylmercury	2.74E-06	0.0051	0.00728	2.2	0.231	0.100	1.00	0.05	0.019	0.50	0.20 (b)	0.35	0.425	0.00	0.107	0.10	0.104	0.03	6.02E-02	0.060	**1.0**

Notes:

PREPARED BY/DATE: MKB 5/17/11
CHECKED BY/DATE: NSR 5/20/11

(a) EDD (mg/kg·day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)]
+ (IRW x CW)/BW
(b) Concentration in Forage Fish constrained by the little blue heron.

Green highlighted entries represent target concentrations in controlling media needed to achieve the target HQ=1.

TABLE B-3

NOAEL RISK CALCULATIONS - DDTR
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_{AI}	C_{AI} [(a)]	P_{FF}	C_{FF}	P_{PF}	C_{PF}	P_{CR}	C_{CR}	P_{AM}	C_{AM}	P_S	EDD [(b)] (mg/kg-day)	NOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Aquatic Receptors																						
Pied-Billed Grebe	DDTR	1.35E-04	1.4	1.57	0.417	0.404	0.0328	1.00	0.60	0.360	0.20	0.51	0.00	0.532	0.20	1.10	0.00	1.24	0.03	2.38E-01	0.227	**1.0**
Belted Kingfisher (Maximum Exposure)	DDTR	1.35E-04	1.4	1.57	0.152	0.566	0.017	1.00	0.00	0.360	1.00	0.42	0.00	0.532	0.00	1.10	0.00	1.24	0.00	2.38E-01	0.227	**1.0**
Belted Kingfisher (Central Tendency)	DDTR	1.35E-04	1.4	1.57	0.152	0.566	0.017	0.50	0.19	0.360	0.51	0.80	0.00	0.532	0.05	1.10	0.25	1.24	0.00	2.38E-01	0.227	**1.0**
Little Blue Heron	DDTR	1.35E-04	1.4	1.57	0.340	0.432	0.160	0.90	0.25	0.360	0.75	0.62	0.00	0.532	0.00	1.10	0.00	1.24	0.03	2.36E-01	0.227	**1.0**
Great Blue Heron	DDTR	1.35E-04	1.4	1.57	2.2	0.231	0.100	1.00	0.05	0.360	0.50	1.29	0.35	0.532	0.00	1.10	0.10	1.24	0.03	2.37E-01	0.227	**1.0**

Notes:

(a) C_{AI} equals 95 UCL of insect data collected July 2010.

(b) EDD (mg/kg·day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)]
+ (IRW x CW)/BW

PREPARED BY/DATE: MKB 5/20/11
CHECKED BY/DATE: NSR 5/25/11

TABLE B-4

NOAEL RISK CALCULATIONS - HCB
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_{AI}	C_{AI}	P_{FF}	C_{FF}	P_{PF}	C_{PF}	P_{CR}	C_{CR}	P_{AM}	C_{AM}	P_{VP}	C_{VP-A}	P_S	EDD [a] (mg/kg-day)	NOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Aquatic Receptors																								
Mink	HCB	3.96E-05	0.38	7.6	0.852	0.134	0.710	1.00	0.00	2.07	0.05	0.469	0.20	0.708	0.10	0.516	0.25	0.0350	0.40	0.286	0.09	1.42E-01	0.137	**1.0**

Notes:

PREPARED BY/DATE: MKB 5/17/11
CHECKED BY/DATE: NSR 5/20/11

(a) EDD (mg/kg-day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)]
+ (IRW x CW)/BW

Aquatic vertebrate prey items used for the mink.

Green highlighted entries represent target concentrations in controlling media needed to achieve the target HQ=1.

TABLE B-5

LOAEL RISK CALCULATIONS - MERCURY
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_{AI}	C_{AI}	P_{FF}	C_{FF}	P_{PF}	C_{PF}	P_{CR}	C_{CR}	P_{AM}	C_{AM}	P_{VP}	$C_{VP,A}$	P_S	EDD [a] (mg/kg-day)	LOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Aquatic Receptors																								
Mink	Mercury	1.69E-04	2.0	27	0.852	0.134	0.710	1.00	0.00	0.046	0.05	0.048	0.20	0.095	0.10	0.077	0.25	0.193	0.40	0.316	0.09	3.69E-01	0.370	**1.0**

Notes:

PREPARED BY/DATE: MKB 5/17/11
CHECKED BY/DATE: NSR 5/20/11

(a) EDD (mg/kg·day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)]
+ (IRW x CW)/BW

Aquatic vertebrate prey items used for the mink.

Green highlighted entries represent target concentrations in controlling media needed to achieve the target HQ=1.

TABLE B-6

LOAEL RISK CALCULATIONS - METHYLMERCURY
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_{AI}	C_{AI}	P_{FF}	C_{FF}	P_{PF}	C_{PF}	P_{CR}	C_{CR}	P_{AM}	C_{AM}	P_S	EDD [a] (mg/kg-day)	LOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Aquatic Receptors																						
Pied-Billed Grebe	Methylmercury	2.74E-06	0.0051	0.00728	0.417	0.404	0.0328	1.00	0.60	0.019	0.20	0.58	0.00	1.495	0.20	0.107	0.00	0.104	0.03	6.02E-02	0.060	**1.0**
Belted Kingfisher (Maximum Exposure)	Methylmercury	2.74E-06	0.0051	0.00728	0.152	0.566	0.017	1.00	0.00	0.019	1.00	0.11	0.00	1.495	0.00	0.107	0.00	0.104	0.00	6.22E-02	0.060	**1.0**
Belted Kingfisher (Central Tendency)	Methylmercury	2.74E-06	0.0051	0.00728	0.152	0.566	0.017	0.50	0.19	0.019	0.51	0.35	0.00	1.495	0.05	0.107	0.25	0.104	0.00	6.04E-02	0.060	**1.0**
Little Blue Heron	Methylmercury	2.74E-06	0.0051	0.00728	0.340	0.432	0.160	0.90	0.25	0.019	0.75	0.20	0.00	1.495	0.00	0.107	0.00	0.104	0.03	6.03E-02	0.060	**1.0**
Great Blue Heron	Methylmercury	2.74E-06	0.0051	0.00728	2.2	0.231	0.100	1.00	0.05	0.019	0.50	0.20 (b)	0.35	0.425	0.00	0.107	0.10	0.104	0.03	6.02E-02	0.060	**1.0**

Notes:

PREPARED BY/DATE: MKB 5/17/11
CHECKED BY/DATE: NSR 5/20/11

(a) EDD (mg/kg·day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)]
+ (IRW x CW)/BW
(b) Concentration in Forage Fish constrained by the little blue heron.
Green highlighted entries represent target concentrations in controlling media needed to achieve the target HQ=1.

TABLE B-7

LOAEL RISK CALCULATIONS - DDTR
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_{AI}	C_{AI} [(a)]	P_{FF}	C_{FF}	P_{PF}	C_{PF}	P_{CR}	C_{CR}	P_{AM}	C_{AM}	P_S	EDD [(b)] (mg/kg-day)	LOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Aquatic Receptors																						
Pied-Billed Grebe	DDTR	1.35E-04	1.4	1.57	0.417	0.404	0.0328	1.00	0.60	0.360	0.20	1.20	0.00	0.532	0.20	1.10	0.00	1.244	0.03	2.94E-01	0.281	**1.0**
Belted Kingfisher (Maximum Exposure)	DDTR	1.35E-04	1.4	1.57	0.152	0.566	0.0170	1.00	0.00	0.360	1.00	0.52	0.00	0.532	0.00	1.10	0.00	1.244	0.00	2.94E-01	0.281	**1.0**
Belted Kingfisher (Central Tendency)	DDTR	1.35E-04	1.4	1.57	0.152	0.566	0.0170	0.50	0.19	0.360	0.51	1.19	0.00	0.532	0.05	1.10	0.25	1.244	0.00	2.95E-01	0.281	**1.0**
Little Blue Heron	DDTR	1.35E-04	1.4	1.57	0.340	0.432	0.160	0.90	0.25	0.360	0.75	0.82	0.00	0.532	0.00	1.10	0.00	1.244	0.03	2.94E-01	0.281	**1.0**
Great Blue Heron	DDTR	1.35E-04	1.4	1.57	2.2	0.231	0.100	1.00	0.05	0.360	0.50	1.78	0.35	0.532	0.00	1.10	0.10	1.244	0.03	2.94E-01	0.281	**1.0**

Notes:

PREPARED BY/DATE: MKB 5/20/11
CHECKED BY/DATE: NSR 5/25/11

(a) C_{AI} equals 95 UCL of insect data collected July 2010.

(b) EDD (mg/kg·day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)]
+ (IRW x CW)/BW

TABLE B-8

LOAEL RISK CALCULATIONS - HCB
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_{AI}	C_{AI}	P_{FF}	C_{FF}	P_{PF}	C_{PF}	P_{CR}	C_{CR}	P_{AM}	C_{AM}	P_{VP}	$C_{VP,A}$	P_S	EDD [a] (mg/kg-day)	LOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Aquatic Receptors																								
Mink	HCB	3.96E-05	0.38	7.6	0.852	0.134	0.71	1.00	0.00	2.073	0.05	0.469	0.20	0.708	0.10	0.516	0.25	0.035	0.40	0.286	0.09	0.142	0.137	**1.0**

Notes:

PREPARED BY/DATE: MKB 5/17/11
CHECKED BY/DATE: NSR 5/20/11

(a) EDD (mg/kg·day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)]
+ (IRW x CW)/BW
Aquatic vertebrate prey items used for the mink.

Green highlighted entries represent target concentrations in controlling media needed to achieve the target HQ=1.

APPENDIX C

SERAFM Model Inputs and Outputs

Scenario 1 – Belted Kingfisher

Diet Comprised of 100% Trophic Level 3 Fish

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	-29.48965936
MeHg	7.33E-08	g/m3	0.07332	31.2197083

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27 ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio				
HgII	7,182,936	1		
MeHg	15,887	1		
Kd_bio				
HgII	127,696,640	1		
MeHg	2,581,565	1		
Kd_DOC				
HgII	301,427	1		
MeHg	310,000	1		
	PCT ERROR	CLEANUP		
MeHg Filtered	3.46	4.22		
HgT Filtered	-61.23			
MeHg Unfilter	-0.92			
HgT Unfiltere	-59.26			

Exposure Concentrations

		Scenario 1 With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2 Background Conditions		Scenario 3 Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.61	ng/L		-15.61	-100	0.47	ng/L	2.19	ng/L
	HgII Filtered	2.99	ng/L		-2.99	-100	0.09	ng/L	0.42	ng/L
Epilimnion	MeHg Filtered	0.46	ng/L	0.47525	0.02	3.4600979	0.07	ng/L	0.11	ng/L
	HgT Filtered	19.07	ng/L	7.39	-11.68	-61.23396	0.63	ng/L	2.72	ng/L
	Hg0 Unfiltered	15.61	ng/L		-15.61	-100	0.47	ng/L	2.19	ng/L
	HgII Unfiltered	88.25	ng/L		-88.25	-100	2.69	ng/L	12.39	ng/L
	MeHg Unfiltered	0.89	ng/L	0.88225	-0.01	-0.923906	0.14	ng/L	0.22	ng/L
	HgT Unfiltered	104.75	ng/L	42.67625	-62.08	-59.26087	3.30	ng/L	14.80	ng/L
Hypolimnion	Hg0 Filtered	26.93	ng/L		-26.93	-100	0.46	ng/L	3.46	ng/L
	HgII Filtered	107.30	ng/L		-107.30	-100	1.65	ng/L	13.63	ng/L
	MeHg Filtered	2.40	ng/L		-2.40	-100	0.18	ng/L	0.43	ng/L
	HgT Filtered	136.63	ng/L		-136.63	-100	2.29	ng/L	17.52	ng/L
	Hg0 Unfiltered	26.93	ng/L		-26.93	-100	0.46	ng/L	3.46	ng/L
	HgII Unfiltered	669.61	ng/L		-669.61	-100	10.31	ng/L	85.07	ng/L
	MeHg Unfiltered	2.64	ng/L		-2.64	-100	0.20	ng/L	0.47	ng/L
	HgT Unfiltered	699.18	ng/L		-699.18	-100	10.96	ng/L	89.00	ng/L
	Sediment									
	Hg0 porewater	26.93	ng/L		-26.93	-100	0.46	ng/L	3.462	ng/L
	HgII porewater	73.21	ng/L		-73.21	-100	1.10	ng/L	9.276	ng/L
	MeHg porewater	0.91	ng/L		-0.91	-100	0.04	ng/L	0.142	ng/L
	HgT porewater	101.06	ng/L		-101.06	-100	1.60	ng/L	12.880	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.26	ug/g		-33.26	-100	0.27	ug/g	4.21	ug/g
	MeHg bulk, dry	0.00827	ug/g	0.00422	0.00	-48.97966	0.00	ug/g	0.00	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.499	ug/g	4.22	ug/g
	Trophic Level 3	0.42	ug/g		-0.42	-100	0.064	ug/g	0.10	ug/g
	Trophic Level 4	0.91	ug/g		-0.91	-100	0.140	ug/g	0.23	ug/g
	HI	4.01					0.61		1.00	
	Sensitive Indicator	Kingfisher					Kingfisher		Kingfisher	
	Target C_sed, dry	4.22	ug/g	Note: 8						
	Target C_sed, wet	1.90	ug/g							

Rate Constants

Process	Media	Value	Units		
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		ratio Sed
1.00E-03	Sediment	1.16E-07	per day		Meth/demeth
Demethylation	Epilimnion	1.16E-08	per day		50.00%
1.00E-03	Hypolimnion	1.16E-07	per day		
2.00E-03	Sediment	2.33E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

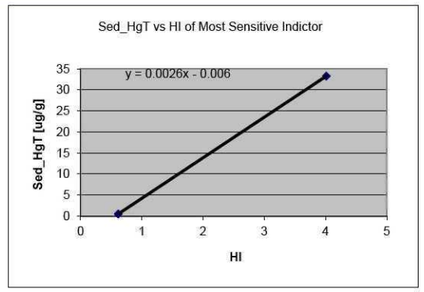
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.51	0.08	0.13
Otter	0.55	0.08	0.14
Mink	**1.07**	0.16	0.27
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.98	0.15	0.25
Kingfisher	**4.01**	0.61	**1.00**
Wood Duck	0.38	0.06	0.10
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
4.01	33.27
0.61	0.50
m =	9.647
b=	-5.431
Sed_HgT	4.215
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.46	0.07	0.114	ng/L

Biota

Trophic Level 1: Phytoplankton	0.09	0.01	0.02	ug Hg/ g wet weight
Trophic Level 2: Insects	0.08	0.01	0.02	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.02	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.42	0.06	0.10	ug Hg/ g wet weight
Trophic Level 4: Bass	0.91	0.14	0.23	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.50	0.08	0.12	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.09	0.01	0.02	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.02	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + (drinking\ rate \bullet [Hg]_{water})$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Wildlife Specific Parameters									Contaminated Sediment Calculations								
Animal	Body Weight [kg in wet weight]	Ingestion Rate [kg wet weight/d]	Drinking rate [L/d]	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants --	Percent of Diet from Trophic Level 2 : Insects --	Percent of Diet from Trophic Level 2 : Crayfish or Frogs --	Percent of Diet from Trophic Level 3 : Fish --	Percent of Diet from Trophic Level 4 : Fish --	Percent of Diet from nonaquatic sources --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	39	0	0	0	39	75	0.51
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	31	9	41	75	0.55
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	74	81	75	1.07
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	19	7	34	0	59	60	0.98
Kingfisher	0.15	0.086	0.017	0%	0%	0%	100%	0%	0%	0	0	0	0	241	0	241	60	4.01
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	18	5	0	0	0	23	60	0.38
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	9	5000	0.00
Human	Human Specific Parameters																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

APPEDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Belted Kingfigher - Diet Comprised of 100% Trophic Level 2 Fish

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.011	0.00	5.91	0.00	0.00	0.00	6	75	0.08
0.006	0.00	0.00	0.19	4.78	1.39	6	75	0.08
0.007	0.00	0.00	0.60	0.43	11.32	12	75	0.16
0.003	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.033	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.005	0.00	2.84	1.02	5.18	0.00	9	60	0.15
0.008	0.00	0.00	0.00	36.89	0.00	37	60	0.61
0.005	2.72	0.80	0.00	0.00	0.00	4	60	0.06
0.000	0.00	0.00	0.07	0.17	1.07	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.018	0.00	9.61	0.00	0.00	0.00	10	75	0.13
0.010	0.00	0.00	0.31	7.77	2.26	10	75	0.14
0.011	0.00	0.00	0.97	0.70	18.42	20	75	0.27
0.005	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.054	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.008	0.00	4.62	1.66	8.43	0.00	15	60	0.25
0.013	0.00	0.00	0.00	60.00	0.00	60	60	1.00
0.008	4.42	1.30	0.00	0.00	0.00	6	60	0.10
0.000	0.00	0.00	0.12	0.28	1.75	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

this table does not all correspond to EPA Report to Congress - check!

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	
HgII	Mean	58,000	50000	100,000	200,000	
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000		
MeHg	Mean	7000	3000	100,000	500,000	
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000		
Hg0		1,000	1,000	3000	1,000	NTG added these 11/1/19

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report.

3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.73E-07	0.47
C_HgII_1_Aq			g/m3	9.11E-08	0.09
C_MeHg_1_Aq			g/m3	7.04E-08	0.07
C_Hg0_2_Aq			g/m3	4.60E-07	0.46
C_HgII_2_Aq			g/m3	1.65E-06	1.65
C_MeHg_2_Aq			g/m3	1.79E-07	0.18
C_Hg0_pore			g/m3	4.60E-07	0.46
C_HgII_pore			g/m3	1.10E-06	1.10
C_MeHg_pore			g/m3	4.38E-08	0.04
C_HgT_1_filtered			g/m3	6.34E-07	0.63
C_HgT_2_filtered			g/m3	2.29E-06	2.29
C_HgT_Sed_filtered			g/m3	1.60E-06	1.60
C_Hg0_1_T			g/m3	4.73E-07	0.47
C_HgII_1_T			g/m3	2.69E-06	2.69
C_MeHg_1_T			g/m3	1.36E-07	0.14
C_Hg0_2_T			g/m3	4.60E-07	0.46
C_HgII_2_T			g/m3	1.03E-05	10.31
C_MeHg_2_T			g/m3	1.97E-07	0.20
C_Hg0_sed, bulk			g/m3	3.82E-07	0
C_HgII_1_sed, bulk			g/m3	2.25E-01	224,763
C_MeHg_1_sed, bulk			g/m3	1.79E-04	179
C_Hg0_sed, wet			g/g	2.98E-13	0.000
C_HgII_1_sed, wet			g/g	2.69E-07	0.269
C_MeHg_1_sed, wet			g/g	1.32E-14	0.000
C_HgT_sed,wet			g/g	2.69E-07	0.269
C_Hg0_sed, dry weight			g/g	8.47E-13	0.0000
C_HgII_1_sed, dry weight			g/g	4.99E-07	0.4989
C_MeHg_1_sed, dry weight			g/g	3.96E-10	0.0004
C_HgT_1			g/m3	3.30E-06	3.296
C_HgT_2			g/m3	1.10E-05	10.964
C_HgT_Sed, dry weight			g/g	4.99E-07	0.499

			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		4.14%	81.52%	14.34%
Layer 2			1.79%	94.01%	4.19%
Sediments			0.08%	99.92%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V_1	Volume of Layer 1	Aw*z_1	m3	648,711
V_2	Volume of Layer 2	Aw*z_2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.006
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.087
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.028
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.153
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.028
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.429
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.133
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.757

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{d\,C^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHg0} \cdot V_w - kw_{ossd} \cdot V_w - v_{zA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{zB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{d\,C^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{ossd} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{zA} \cdot f^{w,1}_{abioHgII} A_w - v_{zB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{d\,C^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{oIMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorMd} V_w - v_{zA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{zB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{d\,C^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photorMd} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{ossd} V_w - v_{zA} \cdot f^{w,2}_{abiHg0} \cdot A_w - v_{zB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{zw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{zw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rz} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{d\,C^w_{HgII2}}{dt} = +\left[kw_{ossd} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{zA} \cdot f^{w,2}_{abiHgII} A_w - v_{zB} \cdot f^{w,2}_{bioHgII} A_w - R_{zw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{zw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rz} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{d\,C^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{zA} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{zB} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{zw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{d\,C^{sed}_{Hg0}}{dt} = \left[R_{zw} f^{w,2}_{aqHg0} + \left(v_{zA} \cdot f^{w,2}_{abioHg0} + v_{zB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{zw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rz} + v_b) \cdot f^{sed}_{sed,Hg0} \cdot A_w - kb_{ossd} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{d\,C^{sed}_{HgII}}{dt} = \left[R_{zw} f^{w,2}_{aqHgII} + \left(v_{zA} \cdot f^{w,2}_{abioHgII} + v_{zB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{ossd} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{zw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rz} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{d\,C^{sed}_{MeHg}}{dt} = \left[R_{zw} f^{w,2}_{aqMeHg} + \left(v_{zA} \cdot f^{w,2}_{abioMeHg} + v_{zB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{zw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rz} + v_b) \cdot f^{sed}_{sed,MeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+08	0.00E+00	0.00E+00	-5.25E+03	1.18E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03

A*x=b

Matrix b

C_Hg0_1_T	-4.89E-01
C_HgII_1_T	-6.18E+01
C_MeHg_1_T	-1.43E+00
C_Hg0_2_T	0.00E+00
C_HgII_2_T	0.00E+00
C_MeHg_2_T	0.00E+00
C_Hg0_sed	0.00E+00
C_HgII_1_sed	0.00E+00
C_MeHg_1_sed	0.00E+00

Solution Matrix

C_Hg0_1_T	4.728E-07
C_HgII_1_T	2.687E-06
C_MeHg_1_T	1.365E-07
C_Hg0_2_T	4.599E-07
C_HgII_2_T	1.031E-05
C_MeHg_2_T	1.965E-07
C_Hg0_sed	3.817E-07
C_HgII_1_sed	2.248E-01
C_MeHg_1_sed	1.785E-04

Inverted Matrix

-8.15E-09	-7.51E-09	-3.03E-09	-7.64E-09	-7.52E-09	-3.06E-09	-7.64E-09	-7.52E-09	-3.06E-09
-3.41E-08	-4.29E-08	-1.27E-08	-4.09E-08	-4.25E-08	-1.29E-08	-4.09E-08	-4.25E-08	-1.29E-08
-1.47E-10	-1.83E-10	-8.72E-08	-3.23E-10	-3.65E-10	-8.66E-08	-3.23E-10	-3.75E-10	-8.66E-08
-6.306E-09	-7.327E-09	-2.510E-09	-4.49E-08	-1.32E-08	-2.79E-09	-4.49E-08	-1.32E-08	-2.79E-09
-1.324E-07	-1.645E-07	-4.994E-08	-2.90E-07	-3.28E-07	-5.15E-08	-2.90E-07	-3.28E-07	-5.16E-08
-4.770E-10	-5.926E-10	-1.113E-07	-1.04E-09	-1.18E-09	-2.80E-07	-1.04E-09	-1.21E-09	-2.80E-07
-5.23E-09	-6.08E-09	-2.08E-09	-3.73E-08	-1.09E-08	-2.31E-09	-3.24E-06	-1.09E-08	-2.31E-09
-2.89E-03	-3.59E-03	-1.09E-03	-6.32E-03	-7.14E-03	-1.12E-03	-6.32E-03	-7.33E-03	-1.13E-03
-6.94E-07	-8.62E-07	-8.71E-05	-1.52E-06	-1.72E-06	-2.19E-04	-1.52E-06	-1.76E-06	-4.07E-04

x=b/A

4.72774E-07	1.36458E-07	4.59867E-07	1.03079E-05	1.96543E-07	3.8169E-07	0.224762892	0.000178549	

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.006
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.039
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.093
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.744
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.123
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.037
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.800
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.090
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		4.06E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		2.04E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01

Rate Constants

kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
e_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43

Effective Partition Coefficients for each Hg species and layer

K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2]\left[H^+\right]^2}{[Hg^{2+}]} = 10^{-4.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{dff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{oo}^{j}C_{oo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{oo}^{j}}}{C_{dis,i}^{j}+C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.61
C_HgII_1_Aq			g/m3	2.99E-06	2.99
C_MeHg_1_Aq			g/m3	4.59E-07	0.46
C_Hg0_2_Aq			g/m3	2.69E-05	26.93
C_HgII_2_Aq			g/m3	1.07E-04	107.30
C_MeHg_2_Aq			g/m3	2.40E-06	2.40
C_Hg0_pore			g/m3	2.69E-05	26.93
C_HgII_pore			g/m3	7.32E-05	73.21
C_MeHg_pore			g/m3	9.14E-07	0.91
C_HgT_1_filtered			g/m3	1.91E-05	19.07
C_HgT_2_filtered			g/m3	1.37E-04	136.63
C_HgT_Sed_filtered			g/m3	1.01E-04	101.06
C_Hg0_1_T			g/m3	1.56E-05	15.61
C_HgII_1_T			g/m3	8.83E-05	88.25
C_MeHg_1_T			g/m3	8.90E-07	0.89
C_Hg0_2_T			g/m3	2.69E-05	26.93
C_HgII_2_T			g/m3	6.70E-04	669.61
C_MeHg_2_T			g/m3	2.64E-06	2.64
C_Hg0_sed			g/m3	2.24E-05	22.35
C_HgII_1_sed			g/m3	1.50E+01	14984386.47
C_MeHg_1_sed			g/m3	3.73E-03	3726.18
C_Hg0_sed, wet			g/g	8.44E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.702
C_MeHg_1_sed, wet			g/g	4.46E-09	0.004
C_HgT_sed,wet			g/g	1.17E-05	11.706
C_Hg0_sed, dry weight			g/g	4.96E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.33E-05	33.26
C_MeHg_1_sed, dry weight			g/g	8.27E-09	0.01
C_HgT_1			g/m3	1.05E-04	104.75
C_HgT_2			g/m3	6.99E-04	699.18
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		0.85%	84.25%	14.90%
Layer 2			0.38%	95.77%	3.85%
Sediments			0.02%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.58263%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.65526%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	2.75205%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	2.80992%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	42.93010%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	13.27265%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.04824%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed	Matrix b	
	1	2	3	4	5	6	7	8	9	b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed

C_T_sed 14.988135 g/m3

Solution Matrix	Inverted Matrix										x=b/A
1.561E-05	-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	1.56E-05	
8.825E-05	-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	8.83E-05	
8.905E-07	-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-16	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	8.9E-07	
2.693E-05	-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	2.69E-05	
6.696E-04	-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.00067	
2.635E-06	-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	2.64E-06	
2.235E-05	-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	2.24E-05	
1.498E+01	9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	14.98439	
3.726E-03	-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.003726	

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	564.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

v_sA	abiotic settling velocity		m/yr	4792.628412
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	13900.95
TSS_1			mg/L	1.80
TSS+2			mg/L	0.43
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2		L/kg	1.58E+07
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.21E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	2.32E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{sw,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	2.19E-06	2.19
C_HgII_1_Aq			g/m3	4.20E-07	0.42
C_MeHg_1_Aq			g/m3	1.14E-07	0.11
C_Hg0_2_Aq			g/m3	3.46E-06	3.46
C_HgII_2_Aq			g/m3	1.36E-05	13.63
C_MeHg_2_Aq			g/m3	4.30E-07	0.43
C_Hg0_pore			g/m3	3.46E-06	3.46
C_HgII_pore			g/m3	9.28E-06	9.28
C_MeHg_pore			g/m3	1.42E-07	0.14
C_HgT_1_filtered			g/m3	2.72E-06	2.72
C_HgT_2_filtered			g/m3	1.75E-05	17.52
C_HgT_Sed_filtered			g/m3	1.29E-05	12.88
C_Hg0_1_T			g/m3	2.19E-06	2.19
C_HgII_1_T			g/m3	1.24E-05	12.39
C_MeHg_1_T			g/m3	2.22E-07	0.22
C_Hg0_2_T			g/m3	3.46E-06	3.46
C_HgII_2_T			g/m3	8.51E-05	85.07
C_MeHg_2_T			g/m3	4.73E-07	0.47
C_Hg0_sed			g/m3	2.87E-06	2.87
C_HgII_1_sed			g/m3	1.90E+00	1,898,394.98
C_MeHg_1_sed			g/m3	5.81E-04	580.82
C_Hg0_sed, wet			g/g	1.08E-12	0.00
C_HgII_1_sed, wet			g/g	1.48E-06	1.48
C_MeHg_1_sed, wet			g/g	6.96E-10	0.00
C_HgT_sed,wet			g/g	1.48E-06	1.48
C_Hg0_sed, dry weight			g/g	6.38E-12	0.00
C_HgII_1_sed, dry weight			g/g	4.21E-06	4.21
C_MeHg_1_sed, dry weight			g/g	1.29E-09	0.00
C_HgT_1			g/m3	1.48E-05	14.80
C_HgT_2			g/m3	8.90E-05	89.00
C_HgT_Sed, dry weight			g/g	4.22E-06	4.22
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		1.50%	83.71%	14.79%
Layer 2			0.53%	95.58%	3.89%
Sediments			0.03%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.58263%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.65526%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75205%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			15.26449%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			2.80992%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			42.93010%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			13.27265%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			75.71189%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photoredl} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoredd} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photoredd} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot A_w \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{med2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoredd} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	2.190E-06
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	1.239E-05
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.42E+00	C_MeHg_1_T	2.220E-07
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	3.462E-06
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	8.507E-05
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	5.30E+03	0.00E+00	0.00E+00	C_MeHg_2_T	4.731E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	2.873E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.90E+00	C_HgII_1_sed	1.898E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed	5.808E-04

A*x=b

Target C_sed, wet 1.898978673 g/g

Inverted Matrix x=b/A

-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	2.2E-06
-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	1.2E-05
-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-16	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	2.2E-07
-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	3.5E-06
-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	8.5E-05
-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	4.7E-07
9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	2.9E-06
9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	1.89839
-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.00058

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	134.70
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	122.63
kw_red_2	water column reduction rate constant	per yr	23.27
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for	per yr	0.82
kw_mer	water column *mer* cleavage demethy	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeH(	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed} \cdot 3.1536x10^7}{z_{sed}}$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{C_{diss,i}^j + C_{DOC,i}^j} \Big/ \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.58263%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75205%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.65526%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.80992%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			13.27265%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			42.93010%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.56114%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			3.93251%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01844%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.29998%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			74.39982%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.34651%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			80.04279%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			3.70796%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.97965%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.17
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.23
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	1,430.88
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Belted Kingfisher - Diet Comprised 100% of Trophic Level 3 Fish

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1	TSS_1	1.80	mg/L	
Sbio_zoo,1	0.5	TSS_2	0.43	mg/L	
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	1.66E-01				
Sbio_dead,2	2.28E-01				
S_abio, sed	8.42E+04				
S_bio_dead,sed	1.43E+03				
S_sed,total	8.57E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b									
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	7.10E+06	S_bio_dead,1	1.66E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.165948
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	2.28E-01	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	0.227765
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	1.43E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	1430.879

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

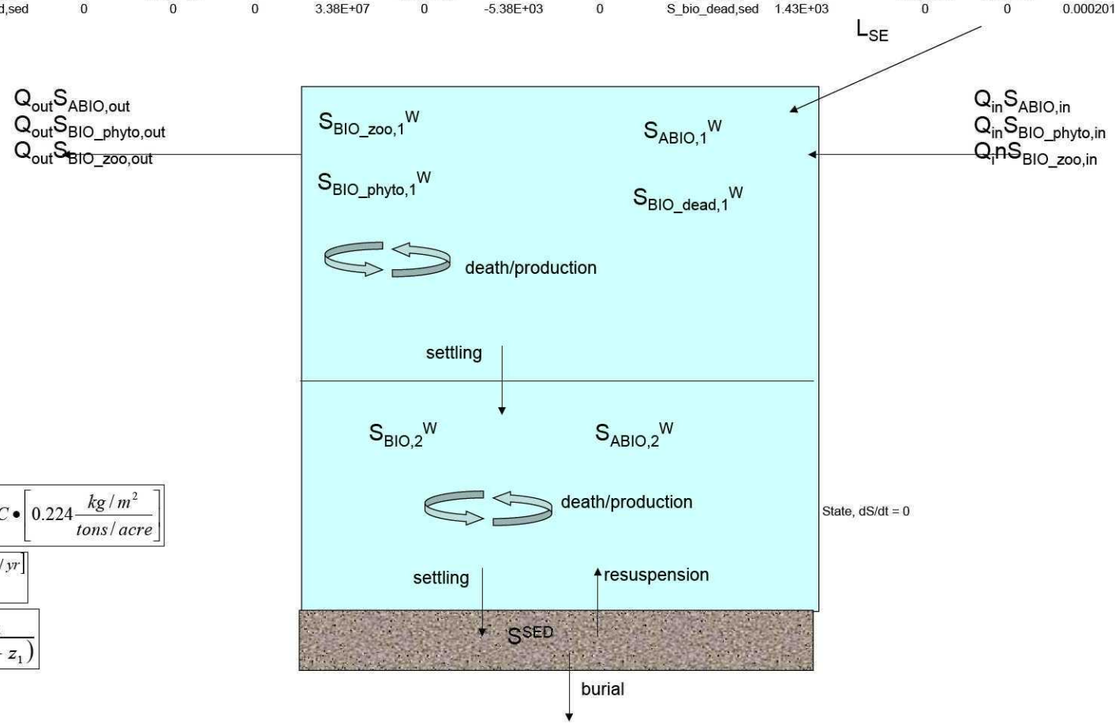
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)	50-300	250-1000	>1000	<50-500
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00583	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.02752		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.02810		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.13273		
k_meth_1	abiotic methylation in layer 1		per yr	2.47E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	6.81E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			5.83E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.81E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.33E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	1.44E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	6.81E-06	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

1 UV-B is modeled as being 0.5% of visible light.
check?

1 $$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location	
East	YES
West	NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Belted Kingfisher

Varied Diet

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	-29.48965936
MeHg	7.33E-08	g/m3	0.07332	31.2197083

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27 ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

		PCT ERROR	CLEANUP
Kd_abio			
HgII	7,182,936	1	
MeHg	15,887	1	
Kd_bio			
HgII	127,696,640	1	
MeHg	2,581,565	1	
Kd_DOC			
HgII	301,427	1	
MeHg	310,000	1	
MeHg Filtered	3.46	14.78	
HgT Filtered	-61.23		
MeHg Unfilter	-0.92		
HgT Unfiltere	-59.26		

Exposure Concentrations

		Scenario 1 With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2 Background Conditions		Scenario 3 Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.61	ng/L		-15.61	-100	0.47	ng/L	7.07	ng/L
	HgII Filtered	2.99	ng/L		-2.99	-100	0.09	ng/L	1.36	ng/L
Epilimnion	MeHg Filtered	0.46	ng/L	0.47525	0.02	3.4600979	0.07	ng/L	0.24	ng/L
	HgT Filtered	19.07	ng/L	7.39	-11.68	-61.23396	0.63	ng/L	8.67	ng/L
	Hg0 Unfiltered	15.61	ng/L		-15.61	-100	0.47	ng/L	7.07	ng/L
	HgII Unfiltered	88.25	ng/L		-88.25	-100	2.69	ng/L	39.98	ng/L
	MeHg Unfiltered	0.89	ng/L	0.88225	-0.01	-0.923906	0.14	ng/L	0.47	ng/L
	HgT Unfiltered	104.75	ng/L	42.67625	-62.08	-59.26087	3.30	ng/L	47.52	ng/L
Hypolimnion	Hg0 Filtered	26.93	ng/L		-26.93	-100	0.46	ng/L	12.00	ng/L
	HgII Filtered	107.30	ng/L		-107.30	-100	1.65	ng/L	47.71	ng/L
	MeHg Filtered	2.40	ng/L		-2.40	-100	0.18	ng/L	1.15	ng/L
	HgT Filtered	136.63	ng/L		-136.63	-100	2.29	ng/L	60.85	ng/L
	Hg0 Unfiltered	26.93	ng/L		-26.93	-100	0.46	ng/L	12.00	ng/L
	HgII Unfiltered	669.61	ng/L		-669.61	-100	10.31	ng/L	297.70	ng/L
	MeHg Unfiltered	2.64	ng/L		-2.64	-100	0.20	ng/L	1.26	ng/L
	HgT Unfiltered	699.18	ng/L		-699.18	-100	10.96	ng/L	310.96	ng/L
	Sediment									
	Hg0 porewater	26.93	ng/L		-26.93	-100	0.46	ng/L	11.999	ng/L
	HgII porewater	73.21	ng/L		-73.21	-100	1.10	ng/L	32.534	ng/L
	MeHg porewater	0.91	ng/L		-0.91	-100	0.04	ng/L	0.423	ng/L
	HgT porewater	101.06	ng/L		-101.06	-100	1.60	ng/L	44.956	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.26	ug/g		-33.26	-100	0.27	ug/g	14.78	ug/g
	MeHg bulk, dry	0.00827	ug/g	0.00422	0.00	-48.97966	0.00	ug/g	0.00	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.499	ug/g	14.78	ug/g
	Trophic Level 3	0.42	ug/g		-0.42	-100	0.064	ug/g	0.22	ug/g
	Trophic Level 4	0.91	ug/g		-0.91	-100	0.140	ug/g	0.48	ug/g
	HI	1.91					0.29		1.00	
	Sensitive Indicator	Kingfisher					Kingfisher		Kingfisher	
	Target C_sed, dry	14.78	ug/g	Note: 8						
	Target C_sed, wet	6.66	ug/g							

Rate Constants

Process		Media	Value	Units		
Methylation		Epilimnion	1.16E-07	per day	1.16E-04	
		Hypolimnion	1.16E-06	per day		ratio Sed
	1.00E-03	Sediment	1.16E-07	per day		Meth/demeth
Demethylation		Epilimnion	1.16E-08	per day		50.00%
	1.00E-03	Hypolimnion	1.16E-07	per day		
	2.00E-03	Sediment	2.33E-07	per day		
Biotic Reduction		Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)		Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light		Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B		Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B		Water Column	58.85	per day per E/m2-day		
Dark Oxidation		Water Column	1.44	per day		

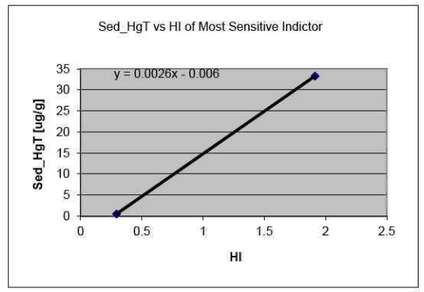
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.51	0.08	0.27
Otter	0.55	0.08	0.29
Mink	**1.07**	0.16	0.56
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.98	0.15	0.51
Kingfisher	**1.91**	0.29	**1.00**
Wood Duck	0.38	0.06	0.20
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
1.91	33.27
0.29	0.50
m =	20.216
b=	-5.431
Sed_HgT	14.784
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.46	0.07	0.240	ng/L

Biota

Trophic Level 1: Phytoplankton	0.09	0.01	0.05	ug Hg/ g wet weight
Trophic Level 2: Insects	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.42	0.06	0.22	ug Hg/ g wet weight
Trophic Level 4: Bass	0.91	0.14	0.48	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.50	0.08	0.26	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.09	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.04	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

	Wildlife Specific Parameters									Contaminated Sediment Calculations								
Animal	**Body Weight** [kg in wet weight]	**Ingestion Rate** [kg wet weight/d]	**Drinking rate** [L/d]	**Percent of Diet from Trophic Level 1 : Phytoplankton and Plants** --	**Percent of Diet from Trophic Level 2 : Insects** --	**Percent of Diet from Trophic Level 2 : Crayfish or Frogs** --	**Percent of Diet from Trophic Level 3 : Fish** --	**Percent of Diet from Trophic Level 4 : Fish** --	**Percent of Diet from nonaquatic sources** --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	39	0	0	0	39	75	0.51
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	31	9	41	75	0.55
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	74	81	75	1.07
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	19	7	34	0	59	60	0.98
Kingfisher	0.15	0.086	0.017	0%	0%	18%	23%	10%	50%	0	0	0	8	54	52	115	60	1.91
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	18	5	0	0	0	23	60	0.38
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	9	5000	0.00
Human	**Human Specific Parameters**																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.011	0.00	5.91	0.00	0.00	0.00	6	75	0.08
0.006	0.00	0.00	0.19	4.78	1.39	6	75	0.08
0.007	0.00	0.00	0.60	0.43	11.32	12	75	0.16
0.003	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.033	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.005	0.00	2.84	1.02	5.18	0.00	9	60	0.15
0.008	0.00	0.00	1.27	8.30	8.03	18	60	0.29
0.005	2.72	0.80	0.00	0.00	0.00	4	60	0.06
0.000	0.00	0.00	0.07	0.17	1.07	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.038	0.00	20.14	0.00	0.00	0.00	20	75	0.27
0.020	0.00	0.00	0.64	16.29	4.73	22	75	0.29
0.024	0.00	0.00	2.04	1.48	38.59	42	75	0.56
0.011	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.113	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.017	0.00	9.69	3.48	17.67	0.00	31	60	0.51
0.027	0.00	0.00	4.33	28.29	27.38	60	60	**1.00**
0.016	9.27	2.73	0.00	0.00	0.00	12	60	0.20
0.000	0.00	0.00	0.24	0.60	3.66	4	5000	0.00
							RfD	
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Belted Kingfisher - Varied Diet

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Belted Kingfisher - Varied Diet

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.73E-07	0.47
C_HgII_1_Aq			g/m3	9.11E-08	0.09
C_MeHg_1_Aq			g/m3	7.04E-08	0.07
C_Hg0_2_Aq			g/m3	4.60E-07	0.46
C_HgII_2_Aq			g/m3	1.65E-06	1.65
C_MeHg_2_Aq			g/m3	1.79E-07	0.18
C_Hg0_pore			g/m3	4.60E-07	0.46
C_HgII_pore			g/m3	1.10E-06	1.10
C_MeHg_pore			g/m3	4.38E-08	0.04
C_HgT_1_filtered			g/m3	6.34E-07	0.63
C_HgT_2_filtered			g/m3	2.29E-06	2.29
C_HgT_Sed_filtered			g/m3	1.60E-06	1.60
C_Hg0_1_T			g/m3	4.73E-07	0.47
C_HgII_1_T			g/m3	2.69E-06	2.69
C_MeHg_1_T			g/m3	1.36E-07	0.14
C_Hg0_2_T			g/m3	4.60E-07	0.46
C_HgII_2_T			g/m3	1.03E-05	10.31
C_MeHg_2_T			g/m3	1.97E-07	0.20
C_Hg0_sed, bulk			g/m3	3.82E-07	0
C_HgII_1_sed, bulk			g/m3	2.25E-01	224,763
C_MeHg_1_sed, bulk			g/m3	1.79E-04	179
C_Hg0_sed, wet			g/g	2.98E-13	0.000
C_HgII_1_sed, wet			g/g	2.69E-07	0.269
C_MeHg_1_sed, wet			g/g	1.32E-14	0.000
C_HgT_sed,wet			g/g	2.69E-07	0.269
C_Hg0_sed, dry weight			g/g	8.47E-13	0.0000
C_HgII_1_sed, dry weight			g/g	4.99E-07	0.4989
C_MeHg_1_sed, dry weight			g/g	3.96E-10	0.0004
C_HgT_1			g/m3	3.30E-06	3.296
C_HgT_2			g/m3	1.10E-05	10.964
C_HgT_Sed, dry weight			g/g	4.99E-07	0.499

			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		4.14%	81.52%	14.34%
Layer 2			1.79%	94.01%	4.19%
Sediments			0.08%	99.92%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V_1	Volume of Layer 1	Aw*z_1	m3	648,711
V_2	Volume of Layer 2	Aw*z_2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.006
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.087
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.028
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.153
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.028
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.429
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.133
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.757

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{zA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{zB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red,1} \cdot V_w - kw_{met} \cdot V_w - v_{zA} \cdot f^{w,1}_{abioHgII} A_w - v_{zB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{met} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{zA} \cdot f^{w,1}_{abioMeHg} A_w - v_{zB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{zA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{zB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{zw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{zw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{met} \cdot V_w - v_{zA} \cdot f^{w,2}_{abioHgII} A_w - v_{zB} \cdot f^{w,2}_{bioHgII} A_w - R_{zw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{zw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth,2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{zA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{zB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{zw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{zw} f^{w,2}_{aqHg0} + \left(v_{zA} \cdot f^{w,2}_{abioHg0} + v_{zB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{zw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{zw} f^{w,2}_{aqHgII} + \left(v_{zA} \cdot f^{w,2}_{abioHgII} + v_{zB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{zw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{met}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{zw} f^{w,2}_{aqMeHg} + \left(v_{zA} \cdot f^{w,2}_{abioMeHg} + v_{zB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{zw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+08	0.00E+00	0.00E+00	-5.25E+03	1.18E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03

b

C Hg0 1 T	-4.89E-01
C HgII 1 T	-6.18E+01
C MeHg 1 T	-1.43E+00
C Hg0 2 T	0.00E+00
C HgII 2 T	0.00E+00
C MeHg 2 T	5.30E+03
C Hg0 sed	0.00E+00
C HgII 1 sed	1.18E+00
C MeHg 1 sed	-5.31E+03

A*x=b

Matrix

C Hg0 1 T	4.728E-07
C HgII 1 T	2.687E-06
C MeHg 1 T	1.365E-07
C Hg0 2 T	4.599E-07
C HgII 2 T	1.031E-05
C MeHg 2 T	1.965E-07
C Hg0 sed	3.817E-07
C HgII 1 sed	2.248E-01
C MeHg 1 sed	1.785E-04

Solution

Inverted Matrix

-8.15E-09	-7.51E-09	-3.03E-09	-7.64E-09	-7.52E-09	-3.06E-09	-7.64E-09	-7.52E-09	-3.06E-09	4.72774E-07
-3.41E-08	-4.29E-08	-1.27E-08	-4.09E-08	-4.25E-08	-1.29E-08	-4.09E-08	-4.25E-08	-1.29E-08	2.68676E-06
-1.47E-10	-1.83E-10	-8.72E-08	-3.23E-10	-3.65E-10	-8.66E-08	-3.23E-10	-3.75E-10	-8.66E-08	1.36459E-07
-6.306E-09	-7.327E-09	-2.510E-09	-4.49E-08	-1.32E-08	-2.79E-09	-4.49E-08	-1.32E-08	-2.79E-09	4.59867E-07
-1.324E-07	-1.645E-07	-4.994E-08	-2.90E-07	-3.28E-07	-5.15E-08	-2.90E-07	-3.28E-07	-5.16E-08	1.03079E-05
-4.770E-10	-5.926E-10	-1.113E-07	-1.04E-09	-1.18E-09	-2.80E-07	-1.04E-09	-1.21E-09	-2.80E-07	1.96543E-07
-5.23E-09	-6.08E-09	-2.08E-09	-3.73E-08	-1.09E-08	-2.31E-09	-3.73E-08	-1.09E-08	-2.31E-09	3.8169E-07
-2.89E-03	-3.59E-03	-1.09E-03	-6.32E-03	-7.14E-03	-1.12E-03	-6.32E-03	-7.33E-03	-1.13E-03	0.224762892
-6.94E-07	-8.62E-07	-8.71E-05	-1.52E-06	-1.72E-06	-2.19E-04	-1.52E-06	-1.76E-06	-4.07E-04	0.000178549

x=b/A

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.006
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.039
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.093
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.744
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.123
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.037
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.800
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.090
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		4.06E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		2.04E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \Big/ \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{C_{filtered,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.61
C_HgII_1_Aq			g/m3	2.99E-06	2.99
C_MeHg_1_Aq			g/m3	4.59E-07	0.46
C_Hg0_2_Aq			g/m3	2.69E-05	26.93
C_HgII_2_Aq			g/m3	1.07E-04	107.30
C_MeHg_2_Aq			g/m3	2.40E-06	2.40
C_Hg0_pore			g/m3	2.69E-05	26.93
C_HgII_pore			g/m3	7.32E-05	73.21
C_MeHg_pore			g/m3	9.14E-07	0.91
C_HgT_1_filtered			g/m3	1.91E-05	19.07
C_HgT_2_filtered			g/m3	1.37E-04	136.63
C_HgT_Sed_filtered			g/m3	1.01E-04	101.06
C_Hg0_1_T			g/m3	1.56E-05	15.61
C_HgII_1_T			g/m3	8.83E-05	88.25
C_MeHg_1_T			g/m3	8.90E-07	0.89
C_Hg0_2_T			g/m3	2.69E-05	26.93
C_HgII_2_T			g/m3	6.70E-04	669.61
C_MeHg_2_T			g/m3	2.64E-06	2.64
C_Hg0_sed			g/m3	2.24E-05	22.35
C_HgII_1_sed			g/m3	1.50E+01	14984386.47
C_MeHg_1_sed			g/m3	3.73E-03	3726.18
C_Hg0_sed, wet			g/g	8.44E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.702
C_MeHg_1_sed, wet			g/g	4.46E-09	0.004
C_HgT_sed,wet			g/g	1.17E-05	11.706
C_Hg0_sed, dry weight			g/g	4.96E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.33E-05	33.26
C_MeHg_1_sed, dry weight			g/g	8.27E-09	0.01
C_HgT_1			g/m3	1.05E-04	104.75
C_HgT_2			g/m3	6.99E-04	699.18
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		0.85%	84.25%	14.90%
Layer 2			0.38%	95.77%	3.85%
Sediments			0.02%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.58263%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.65526%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	2.75205%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	2.80992%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	42.93010%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	13.27265%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.04824%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed

A*x=b

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

C T sed 14.988135 g/m3

Solution Matrix	Inverted Matrix										x=b/A
1.561E-05	-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	1.56E-05	
8.825E-05	-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	8.83E-05	
8.905E-07	-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-16	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	8.9E-07	
2.693E-05	-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	2.69E-05	
6.696E-04	-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.00067	
2.635E-06	-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	2.64E-06	
2.235E-05	-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	2.24E-05	
1.498E+01	9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	14.98439	
3.726E-03	-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.003726	

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	564.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	13900.95
TSS_1			mg/L	1.80
TSS+2			mg/L	0.43
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2		L/kg	1.58E+07
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.21E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	2.32E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	7.07E-06	7.07
C_HgII_1_Aq			g/m3	1.36E-06	1.36
C_MeHg_1_Aq			g/m3	2.40E-07	0.24
C_Hg0_2_Aq			g/m3	1.20E-05	12.00
C_HgII_2_Aq			g/m3	4.77E-05	47.71
C_MeHg_2_Aq			g/m3	1.15E-06	1.15
C_Hg0_pore			g/m3	1.20E-05	12.00
C_HgII_pore			g/m3	3.25E-05	32.53
C_MeHg_pore			g/m3	4.23E-07	0.42
C_HgT_1_filtered			g/m3	8.67E-06	8.67
C_HgT_2_filtered			g/m3	6.09E-05	60.85
C_HgT_Sed_filtered			g/m3	4.50E-05	44.96
C_Hg0_1_T			g/m3	7.07E-06	7.07
C_HgII_1_T			g/m3	4.00E-05	39.98
C_MeHg_1_T			g/m3	4.65E-07	0.47
C_Hg0_2_T			g/m3	1.20E-05	12.00
C_HgII_2_T			g/m3	2.98E-04	297.70
C_MeHg_2_T			g/m3	1.26E-06	1.26
C_Hg0_sed			g/m3	9.96E-06	9.96
C_HgII_1_sed			g/m3	6.66E+00	6,658,535.49
C_MeHg_1_sed			g/m3	1.72E-03	1,724.97
C_Hg0_sed, wet			g/g	3.76E-12	0.00
C_HgII_1_sed, wet			g/g	5.20E-06	5.20
C_MeHg_1_sed, wet			g/g	2.07E-09	0.00
C_HgT_sed,wet			g/g	5.20E-06	5.20
C_Hg0_sed, dry weight			g/g	2.21E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.48E-05	14.78
C_MeHg_1_sed, dry weight			g/g	3.83E-09	0.00
C_HgT_1			g/m3	4.75E-05	47.52
C_HgT_2			g/m3	3.11E-04	310.96
C_HgT_Sed, dry weight			g/g	1.48E-05	14.78
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		0.98%	84.14%	14.88%
Layer 2			0.41%	95.74%	3.86%
Sediments			0.03%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.58263%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.65526%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75205%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			15.26449%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			2.80992%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			42.93010%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			13.27265%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			75.71189%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{med2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	7.072E-06
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	3.998E-05
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.42E+00	C_MeHg_1_T	4.651E-07
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.200E-05
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	2.977E-04
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T	1.260E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	9.960E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	6.66E+00	C_HgII_1_sed	6.659E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed	1.725E-03

Inverted Matrix

-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	7.1E-06
-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	4E-05
-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-16	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	4.7E-07
-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	1.2E-05
-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.0003
-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	1.3E-06
-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	1E-05
9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	6.65854
-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.00172

x=b/A

A*x=b

Target C_sed, wet 6.660270428 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	134.70
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	122.63
kw_red_2	water column reduction rate constant	per yr	23.27
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for	per yr	0.82
kw_mer	water column *mer* cleavage demeth	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeH	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \quad \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{}{C_{dissi}^j + C_{DOC,i}^j} \quad \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left(K_{L,i}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.58263%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75205%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.65526%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.80992%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			13.27265%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			42.93010%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.56114%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			3.93251%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01844%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.29998%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			74.39982%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.34651%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			80.04279%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			3.70796%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.97965%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.17
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.23
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	1,430.88
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1	TSS_1	1.80	mg/L	
Sbio_zoo,1	0.5	TSS_2	0.43	mg/L	
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	1.66E-01				
Sbio_dead,2	2.28E-01				
S_abio, sed	8.42E+04				
S_bio_dead,sed	1.43E+03				
S_sed,total	8.57E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

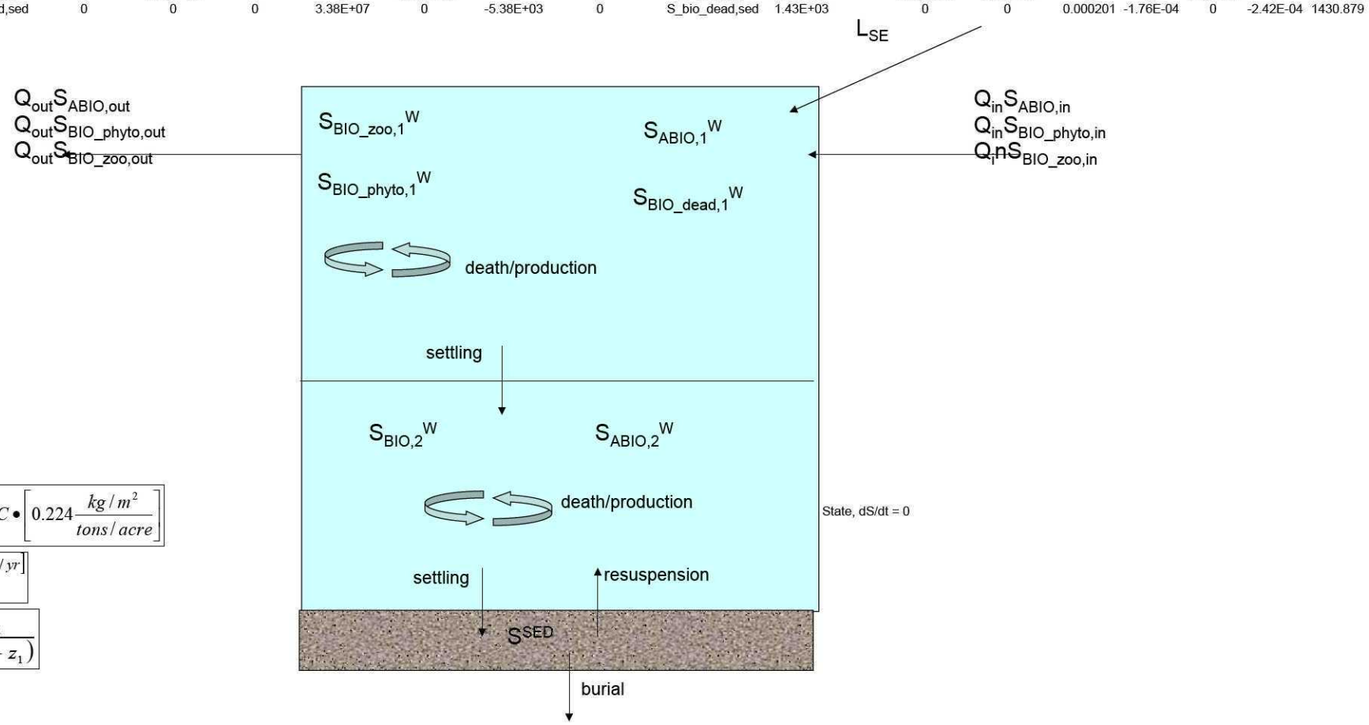
Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b									
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	7.10E+06	S_bio_dead,1	1.66E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.165948
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	2.28E-01	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	0.227765
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	1.43E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	1430.879



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Belted Kingfisher – Varied Diet

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)	50-300	250-1000	>1000	<50-500
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00583	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.02752		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.02810		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.13273		
k_meth_1	abiotic methylation in layer 1		per yr	2.47E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	6.81E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			5.83E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.81E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.33E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	1.44E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	6.81E-06	

$$k_{demeth} = k_{demeth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0	* currently assume no reduction in sediments	
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1	
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02		
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03		
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00		
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01		

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

1 UV-B is modeled as being 0.5% of visible light.
check?

1 $$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Little Blue Heron

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury

Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Kd_abio		
HgII	7,182,936	1
MeHg	15,887	1

Kd_bio		
HgII	127,696,640	1
MeHg	2,581,565	1

Kd_DOC		
HgII	301,427	1
MeHg	310,000	1

	PCT ERROR	CLEANUP
MeHg Filtered	3.46	10.65
HgT Filtered	-61.23	
MeHg Unfilte	-0.92	
HgT Unfiltere	-59.26	

Inflow Mercury Concentrations					
Hg0	0	g/m3			
HgII	5.64E-06	g/m3	5.64	-29.48965936	
MeHg	7.33E-08	g/m3	0.07332	31.2197083	Fish
Total Mercury Concentration in Contaminated Sediment, dry weight	33.27	ug/g			
Known Mercury in Contaminated Soils					
Cs,Hg0	0	g/m3	7		
Cs,HgII	1.129080624	g/m3			
Cs,MeHg	4.13E-03	g/m3			
Required Hazard Index for Sensitive Indicator	1				

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.61	ng/L		-15.61	-100	0.47	ng/L	5.16	ng/L
	HgII Filtered	2.99	ng/L		-2.99	-100	0.09	ng/L	0.99	ng/L
Epilimnion	MeHg Filtered	0.46	ng/L	0.47525	0.02	3.4600979	0.07	ng/L	0.19	ng/L
	HgT Filtered	19.07	ng/L	7.39	-11.68	-61.23396	0.63	ng/L	6.34	ng/L
	Hg0 Unfiltered	15.61	ng/L		-15.61	-100	0.47	ng/L	5.16	ng/L
	HgII Unfiltered	88.25	ng/L		-88.25	-100	2.69	ng/L	29.18	ng/L
	MeHg Unfiltered	0.89	ng/L	0.88225	-0.01	-0.923906	0.14	ng/L	0.37	ng/L
	HgT Unfiltered	104.75	ng/L	42.67625	-62.08	-59.26087	3.30	ng/L	34.71	ng/L
Hypolimnion	Hg0 Filtered	26.93	ng/L		-26.93	-100	0.46	ng/L	8.66	ng/L
	HgII Filtered	107.30	ng/L		-107.30	-100	1.65	ng/L	34.36	ng/L
	MeHg Filtered	2.40	ng/L		-2.40	-100	0.18	ng/L	0.87	ng/L
	HgT Filtered	136.63	ng/L		-136.63	-100	2.29	ng/L	43.89	ng/L
	Hg0 Unfiltered	26.93	ng/L		-26.93	-100	0.46	ng/L	8.66	ng/L
	HgII Unfiltered	669.61	ng/L		-669.61	-100	10.31	ng/L	214.44	ng/L
	MeHg Unfiltered	2.64	ng/L		-2.64	-100	0.20	ng/L	0.95	ng/L
	HgT Unfiltered	699.18	ng/L		-699.18	-100	10.96	ng/L	224.05	ng/L
	Sediment									
	Hg0 porewater	26.93	ng/L		-26.93	-100	0.46	ng/L	8.656	ng/L
	HgII porewater	73.21	ng/L		-73.21	-100	1.10	ng/L	23.427	ng/L
	MeHg porewater	0.91	ng/L		-0.91	-100	0.04	ng/L	0.313	ng/L
	HgT porewater	101.06	ng/L		-101.06	-100	1.60	ng/L	32.396	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.26	ug/g		-33.26	-100	0.27	ug/g	10.64	ug/g
	MeHg bulk, dry	0.00827	ug/g	0.00422	0.00	-48.97966	0.00	ug/g	0.00	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.499	ug/g	10.65	ug/g
	Trophic Level 3	0.42	ug/g		-0.42	-100	0.064	ug/g	0.17	ug/g
	Trophic Level 4	0.91	ug/g		-0.91	-100	0.140	ug/g	0.38	ug/g
	HI	2.41					0.37		1.00	
	Sensitive Indicator	Little Blue Heron					Little Blue Heron		Little Blue Heron	
	Target C_sed, dry	10.65	ug/g	Note: 8						
	Target C_sed, wet	4.80	ug/g							

Rate Constants

Process	Media	Value	Units		
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		ratio Sed
1.00E-03	Sediment	1.16E-07	per day		Meth/demeth
Demethylation	Epilimnion	1.16E-08	per day		50.00%
1.00E-03	Hypolimnion	1.16E-07	per day		
2.00E-03	Sediment	2.33E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

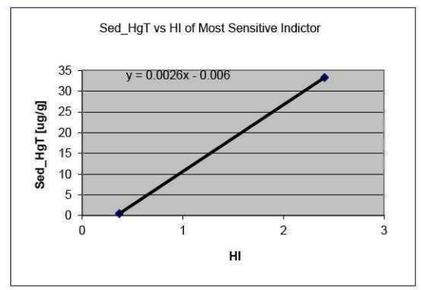
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.51	0.08	0.21
Otter	0.55	0.08	0.23
Mink	**1.07**	0.16	0.45
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	**2.41**	0.37	**1.00**
Pied-bill Grebe	0.98	0.15	0.41
Kingfisher	0.00	0.00	0.00
Wood Duck	0.38	0.06	0.16
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
2.41	33.27
0.37	0.50
m =	16.077
b=	-5.431
Sed_HgT	10.646
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

	Site-Specific User Input	Required
	Model Calculated	No input required
	Data Necessary for certain sites	Only necessary if applicable to site of interest
	Scenario 1 Output	
	Scenario 2 Output	
	Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.46	0.07	0.191	ng/L

Biota

Trophic Level 1: Phytoplankton	0.09	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Insects	0.08	0.01	0.03	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.03	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.42	0.06	0.17	ug Hg/ g wet weight
Trophic Level 4: Bass	0.91	0.14	0.38	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.50	0.08	0.21	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.09	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.03	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

Animal	Body Weight [kg in wet weight]	Ingestion Rate [kg wet weight/d]	Drinking rate [L/d]	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants --	Percent of Diet from Trophic Level 2 : Insects --	Percent of Diet from Trophic Level 2 : Crayfish or Frogs --	Percent of Diet from Trophic Level 3 : Fish --	Percent of Diet from Trophic Level 4 : Fish --	Percent of Diet from nonaquatic sources --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	39	0	0	0	39	75	0.51
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	31	9	41	75	0.55
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	74	81	75	1.07
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	25%	0%	75%	0%	0%	0	0	8	0	136	0	144	60	2.41
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	19	7	34	0	59	60	0.98
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	18	5	0	0	0	23	60	0.38
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	9	5000	0.00

Human

																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution 5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.011	0.00	5.91	0.00	0.00	0.00	6	75	0.08
0.006	0.00	0.00	0.19	4.78	1.39	6	75	0.08
0.007	0.00	0.00	0.60	0.43	11.32	12	75	0.16
0.003	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.033	0.00	1.27	0.00	20.86	0.00	22	60	0.37
0.005	0.00	2.84	1.02	5.18	0.00	9	60	0.15
0.008	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.005	2.72	0.80	0.00	0.00	0.00	4	60	0.06
0.000	0.00	0.00	0.07	0.17	1.07	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.031	0.00	16.02	0.00	0.00	0.00	16	75	0.21
0.016	0.00	0.00	0.51	12.96	3.76	17	75	0.23
0.019	0.00	0.00	1.62	1.17	30.69	33	75	0.45
0.009	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.090	0.00	3.44	0.00	56.56	0.00	60	60	**1.00**
0.014	0.00	7.70	2.77	14.05	0.00	25	60	0.41
0.022	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.013	7.37	2.17	0.00	0.00	0.00	10	60	0.16
0.000	0.00	0.00	0.19	0.47	2.91	4	5000	0.00
							RfD	
0.003	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Little Blue Heron

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Coun	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeHg	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Little Blue Heron

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and reflec		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22 x 10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

this table does not all correspond to EPA Report to Congress - check!

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	
HgII	Mean	58,000	50000	100,000	200,000	
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000		
MeHg	Mean	7000	3000	100,000	500,000	
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000		
Hg0		1,000	1,000	3000	1,000	NTG added these 11/1/19

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)
HgII	mean	3.8	5.3	4.9	5.4
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6
	n	17	35	2	3
MeHg	mean	2.8	4.9	3.9	5
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5
	n	11	2		

Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
			199526.23				
630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	1584893.2	100000	316227.77	8	635462.6		12,679,146
			630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.38

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.73E-07	0.47
C_HgII_1_Aq			g/m3	9.11E-08	0.09
C_MeHg_1_Aq			g/m3	7.04E-08	0.07
C_Hg0_2_Aq			g/m3	4.60E-07	0.46
C_HgII_2_Aq			g/m3	1.65E-06	1.65
C_MeHg_2_Aq			g/m3	1.79E-07	0.18
C_Hg0_pore			g/m3	4.60E-07	0.46
C_HgII_pore			g/m3	1.10E-06	1.10
C_MeHg_pore			g/m3	4.38E-08	0.04
C_HgT_1_filtered			g/m3	6.34E-07	0.63
C_HgT_2_filtered			g/m3	2.29E-06	2.29
C_HgT_Sed_filtered			g/m3	1.60E-06	1.60
C_Hg0_1_T			g/m3	4.73E-07	0.47
C_HgII_1_T			g/m3	2.69E-06	2.69
C_MeHg_1_T			g/m3	1.36E-07	0.14
C_Hg0_2_T			g/m3	4.60E-07	0.46
C_HgII_2_T			g/m3	1.03E-05	10.31
C_MeHg_2_T			g/m3	1.97E-07	0.20
C_Hg0_sed, bulk			g/m3	3.82E-07	0
C_HgII_1_sed, bulk			g/m3	2.25E-01	224,763
C_MeHg_1_sed, bulk			g/m3	1.79E-04	179
C_Hg0_sed, wet			g/g	2.98E-13	0.000
C_HgII_1_sed, wet			g/g	2.69E-07	0.269
C_MeHg_1_sed, wet			g/g	1.32E-14	0.000
C_HgT_sed,wet			g/g	2.69E-07	0.269
C_Hg0_sed, dry weight			g/g	8.47E-13	0.0000
C_HgII_1_sed, dry weight			g/g	4.99E-07	0.4989
C_MeHg_1_sed, dry weight			g/g	3.96E-10	0.0004
C_HgT_1			g/m3	3.30E-06	3.296
C_HgT_2			g/m3	1.10E-05	10.964
C_HgT_Sed, dry weight			g/g	4.99E-07	0.499

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)	4.14%	81.52%	14.34%
Layer 2		1.79%	94.01%	4.19%
Sediments		0.08%	99.92%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V_1	Volume of Layer 1	Aw*z_1	m3	648,711
V_2	Volume of Layer 2	Aw*z_2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.006
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.087
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.028
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.153
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.028
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.429
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.133
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.757

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{met} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{met} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{met} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth,2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+08	0.00E+00	0.00E+00	-5.25E+03	1.18E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03

b

C Hg0 1 T	-4.89E-01
C HgII 1 T	-6.18E+01
C MeHg 1 T	-1.43E+00
C Hg0 2 T	0.00E+00
C HgII 2 T	0.00E+00
C MeHg 2 T	5.30E+03
C Hg0 sed	0.00E+00
C HgII 1 sed	1.18E+00
C MeHg 1 sed	-5.31E+03

A*x=b

Matrix

C Hg0 1 T	4.728E-07
C HgII 1 T	2.687E-06
C MeHg 1 T	1.365E-07
C Hg0 2 T	4.599E-07
C HgII 2 T	1.031E-05
C MeHg 2 T	1.965E-07
C Hg0 sed	3.817E-07
C HgII 1 sed	2.248E-01
C MeHg 1 sed	1.785E-04

Solution

Inverted Matrix

-8.15E-09	-7.51E-09	-3.03E-09	-7.64E-09	-7.52E-09	-3.06E-09	-7.64E-09	-7.52E-09	-3.06E-09	4.72774E-07
-3.41E-08	-4.29E-08	-1.27E-08	-4.09E-08	-4.25E-08	-1.29E-08	-4.09E-08	-4.25E-08	-1.29E-08	2.68676E-06
-1.47E-10	-1.83E-10	-8.72E-08	-3.23E-10	-3.65E-10	-8.66E-08	-3.23E-10	-3.75E-10	-8.66E-08	1.36459E-07
-6.306E-09	-7.327E-09	-2.510E-09	-4.49E-08	-1.32E-08	-2.79E-09	-4.49E-08	-1.32E-08	-2.79E-09	4.59867E-07
-1.324E-07	-1.645E-07	-4.994E-08	-2.90E-07	-3.28E-07	-5.15E-08	-2.90E-07	-3.28E-07	-5.16E-08	1.03079E-05
-4.770E-10	-5.926E-10	-1.113E-07	-1.04E-09	-1.18E-09	-2.80E-07	-1.04E-09	-1.21E-09	-2.80E-07	1.96543E-07
-5.23E-09	-6.08E-09	-2.08E-09	-3.73E-08	-1.09E-08	-2.31E-09	-3.73E-08	-1.09E-08	-2.31E-09	3.8169E-07
-2.89E-03	-3.59E-03	-1.09E-03	-6.32E-03	-7.14E-03	-1.12E-03	-6.32E-03	-7.33E-03	-1.13E-03	0.224762892
-6.94E-07	-8.62E-07	-8.71E-05	-1.52E-06	-1.72E-06	-2.19E-04	-1.52E-06	-1.76E-06	-4.07E-04	0.000178549

x=b/A

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.006
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.039
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.093
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.744
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.123
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.037
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.800
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.090
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		4.06E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		2.04E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer.* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer.* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \Big/ \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{C_{dtss,i}^{j}+C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.61
C_HgII_1_Aq			g/m3	2.99E-06	2.99
C_MeHg_1_Aq			g/m3	4.59E-07	0.46
C_Hg0_2_Aq			g/m3	2.69E-05	26.93
C_HgII_2_Aq			g/m3	1.07E-04	107.30
C_MeHg_2_Aq			g/m3	2.40E-06	2.40
C_Hg0_pore			g/m3	2.69E-05	26.93
C_HgII_pore			g/m3	7.32E-05	73.21
C_MeHg_pore			g/m3	9.14E-07	0.91
C_HgT_1_filtered			g/m3	1.91E-05	19.07
C_HgT_2_filtered			g/m3	1.37E-04	136.63
C_HgT_Sed_filtered			g/m3	1.01E-04	101.06
C_Hg0_1_T			g/m3	1.56E-05	15.61
C_HgII_1_T			g/m3	8.83E-05	88.25
C_MeHg_1_T			g/m3	8.90E-07	0.89
C_Hg0_2_T			g/m3	2.69E-05	26.93
C_HgII_2_T			g/m3	6.70E-04	669.61
C_MeHg_2_T			g/m3	2.64E-06	2.64
C_Hg0_sed			g/m3	2.24E-05	22.35
C_HgII_1_sed			g/m3	1.50E+01	14984386.47
C_MeHg_1_sed			g/m3	3.73E-03	3726.18
C_Hg0_sed, wet			g/g	8.44E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.702
C_MeHg_1_sed, wet			g/g	4.46E-09	0.004
C_HgT_sed,wet			g/g	1.17E-05	11.706
C_Hg0_sed, dry weight			g/g	4.96E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.33E-05	33.26
C_MeHg_1_sed, dry weight			g/g	8.27E-09	0.01
C_HgT_1			g/m3	1.05E-04	104.75
C_HgT_2			g/m3	6.99E-04	699.18
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		0.85%	84.25%	14.90%
Layer 2			0.38%	95.77%	3.85%
Sediments			0.02%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.58263%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.65526%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	2.75205%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	2.80992%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	42.93010%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	13.27265%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.04824%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{methg} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{methg} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{volHg0} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{methg} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{methg2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed	Matrix b	
	1	2	3	4	5	6	7	8	9		
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix										x=b/A
1.561E-05	-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	1.56E-05	C_Hg0_1_T
8.825E-05	-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	8.83E-05	C_HgII_1_T
8.905E-07	-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-15	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	8.9E-07	C_MeHg_1_T
2.693E-05	-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	2.69E-05	C_Hg0_2_T
6.696E-04	-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.00067	C_HgII_2_T
2.635E-06	-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	2.64E-06	C_MeHg_2_T
2.235E-05	-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	2.24E-05	C_Hg0_sed
1.498E+01	9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	14.98439	C_HgII_1_sed
3.726E-03	-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.003726	C_MeHg_1_sed

C_T_sed 14.988135 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	564.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq\_i}^{sw,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

v_sA	abiotic settling velocity		m/yr	4792.628412
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	13900.95
TSS_1			mg/L	1.80
TSS+2			mg/L	0.43

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

Effective Partition Coefficients for each Hg species and layer		
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for HgII in layer 1	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for HgII in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	5.16E-06	5.16
C_HgII_1_Aq			g/m3	9.90E-07	0.99
C_MeHg_1_Aq			g/m3	1.91E-07	0.19
C_Hg0_2_Aq			g/m3	8.66E-06	8.66
C_HgII_2_Aq			g/m3	3.44E-05	34.36
C_MeHg_2_Aq			g/m3	8.66E-07	0.87
C_Hg0_pore			g/m3	8.66E-06	8.66
C_HgII_pore			g/m3	2.34E-05	23.43
C_MeHg_pore			g/m3	3.13E-07	0.31
C_HgT_1_filtered			g/m3	6.34E-06	6.34
C_HgT_2_filtered			g/m3	4.39E-05	43.89
C_HgT_Sed_filtered			g/m3	3.24E-05	32.40
C_Hg0_1_T			g/m3	5.16E-06	5.16
C_HgII_1_T			g/m3	2.92E-05	29.18
C_MeHg_1_T			g/m3	3.70E-07	0.37
C_Hg0_2_T			g/m3	8.66E-06	8.66
C_HgII_2_T			g/m3	2.14E-04	214.44
C_MeHg_2_T			g/m3	9.52E-07	0.95
C_Hg0_sed			g/m3	7.18E-06	7.18
C_HgII_1_sed			g/m3	4.79E+00	4,794,590.20
C_MeHg_1_sed			g/m3	1.28E-03	1,276.95
C_Hg0_sed, wet			g/g	2.71E-12	0.00
C_HgII_1_sed, wet			g/g	3.74E-06	3.74
C_MeHg_1_sed, wet			g/g	1.53E-09	0.00
C_HgT_sed,wet			g/g	3.75E-06	3.75
C_Hg0_sed, dry weight			g/g	1.59E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.06E-05	10.64
C_MeHg_1_sed, dry weight			g/g	2.83E-09	0.00
C_HgT_1			g/m3	3.47E-05	34.71
C_HgT_2			g/m3	2.24E-04	224.05
C_HgT_Sed, dry weight			g/g	1.06E-05	10.65
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		1.07%	84.07%	14.87%
Layer 2			0.42%	95.71%	3.86%
Sediments			0.03%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.58263%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.65526%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	2.75205%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	2.80992%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	42.93010%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	13.27265%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	75.71189%

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{biaHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHgII} A_w - v_{sB} \cdot f^{w,1}_{biaHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{oIMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{sA} \cdot f^{w,1}_{abiaMeHg} A_w - v_{sB} \cdot f^{w,1}_{biaMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{biaHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiaHgII} A_w - v_{sB} \cdot f^{w,2}_{biaHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiaMeHg} A_w - v_{sB} \cdot f^{w,2}_{biaMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2} + Q' \cdot C^w_{MeHg1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{sA} \cdot f^{w,2}_{abiaHg0} + v_{sB} \cdot f^{w,2}_{biaHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{sA} \cdot f^{w,2}_{abiaHgII} + v_{sB} \cdot f^{w,2}_{biaHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{sA} \cdot f^{w,2}_{abiaMeHg} + v_{sB} \cdot f^{w,2}_{biaMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	5.160E-06	-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	5.16E-06
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	2.918E-05	-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	2.92E-05
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T	3.699E-07	-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-16	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	3.7E-07
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	8.656E-06	-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	8.66E-06
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	2.144E-04	-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.000214
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T	9.517E-07	-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	9.52E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	7.185E-06	-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	7.18E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	4.80E+00	C_HgII_1_sed	4.795E+00	9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	4.79459
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed	1.277E-03	-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.001277

Target C_sed, wet 4.795874337 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate cc	per yr	134.70
kw_v,HgII	water column volatilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatilization loss rate cc	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	122.63
kw_red_2	water column reduction rate constant,	per yr	23.27
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for l	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for l	per yr	0.82
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{ag,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2]\left[H^+\right]^2}{\left[Hg^{2+}\right]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \Big/ \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{C_{diss,i}^j + C_{DOC,i}^j}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = (D_{dry,i} + D_{wet,i}) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.58263%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75205%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.65526%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.80992%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			13.27265%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			42.93010%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.56114%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			3.93251%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01844%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.29998%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			74.39982%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.34651%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			80.04279%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			3.70796%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.97965%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.17
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.23
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	1,430.88

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

DOC_1	Dissolved Organic Carbon Concentration in Layer 1	g/m3	16	
DOC_2	Dissolved Organic Carbon Concentration in Layer 2	g/m3	16	
Symbol	**Parameter**	**Units**	**Value**	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1	TSS_1	1.80	mg/L	
Sbio_zoo,1	0.5	TSS_2	0.43	mg/L	
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	1.66E-01				
Sbio_dead,2	2.28E-01				
S_abio, sed	8.42E+04				
S_bio_dead,sed	1.43E+03				
S_sed,total	8.57E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			
	1	2	3	4	5	6	b	Matrix	
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	7.10E+06	S_bio_dead,1	1.66E-01
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	2.28E-01
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	1.43E+03

Solution Matrix	Matrix Inversion						x=b/A
S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	1.66E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.165948
S_bio_dead,2	2.28E-01	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	0.227765
S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	1.43E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	1430.879

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

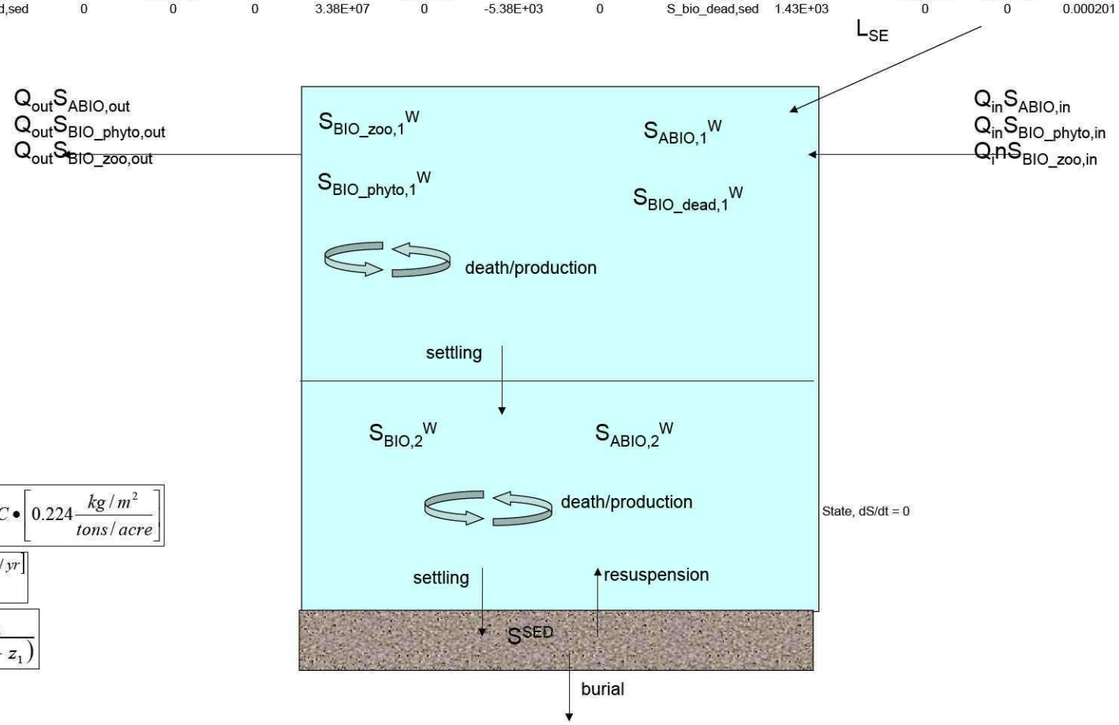
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Little Blue Heron

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00583	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.02752		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.02810		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.13273		
k_meth_1	abiotic methylation in layer 1		per yr	2.47E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	6.81E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			5.83E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.81E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.33E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	1.44E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	6.81E-06	

$$k_{demeth} = k_{demeth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that
only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation
suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability.
Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes
kw_basered	base reduction rate		per day	0.03	2
kw_basered_sed	base reduction rate in sediments		per day	0	* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00	
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00	
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02	
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02	
kb_red	abiotic reduction in sediment		per day	0.00E+00	
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
kb_red	abiotic reduction in sediment		per yr	0.00	

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s

2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

1 UV-B is modeled as being 0.5% of visible light.
check?

1

$$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV-B} = 0.4415 * (DOC)^{.86}$$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location	
East	YES
West	NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Great Blue Heron

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	-29.48965936
MeHg	7.33E-08	g/m3	0.07332	31.2197083

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27 ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio				
HgII	7,182,936	1		
MeHg	15,887	1		
Kd_bio				
HgII	127,696,640	1		
MeHg	2,581,565	1		
Kd_DOC				
HgII	301,427	1		
MeHg	310,000	1		
	PCT ERROR	CLEANUP		
MeHg Filtered	3.46	13.09		
HgT Filtered	-61.23			
MeHg Unfilter	-0.92			
HgT Unfiltere	-59.26			

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.61	ng/L		-15.61	-100	0.47	ng/L	6.29	ng/L
	HgII Filtered	2.99	ng/L		-2.99	-100	0.09	ng/L	1.21	ng/L
Epilimnion	MeHg Filtered	0.46	ng/L	0.47525	0.02	3.4600979	0.07	ng/L	0.22	ng/L
	HgT Filtered	19.07	ng/L	7.39	-11.68	-61.23396	0.63	ng/L	7.71	ng/L
	Hg0 Unfiltered	15.61	ng/L		-15.61	-100	0.47	ng/L	6.29	ng/L
	HgII Unfiltered	88.25	ng/L		-88.25	-100	2.69	ng/L	35.55	ng/L
	MeHg Unfiltered	0.89	ng/L	0.88225	-0.01	-0.923906	0.14	ng/L	0.43	ng/L
	HgT Unfiltered	104.75	ng/L	42.67625	-62.08	-59.26087	3.30	ng/L	42.27	ng/L
Hypolimnion	Hg0 Filtered	26.93	ng/L		-26.93	-100	0.46	ng/L	10.63	ng/L
	HgII Filtered	107.30	ng/L		-107.30	-100	1.65	ng/L	42.23	ng/L
	MeHg Filtered	2.40	ng/L		-2.40	-100	0.18	ng/L	1.03	ng/L
	HgT Filtered	136.63	ng/L		-136.63	-100	2.29	ng/L	53.89	ng/L
	Hg0 Unfiltered	26.93	ng/L		-26.93	-100	0.46	ng/L	10.63	ng/L
	HgII Unfiltered	669.61	ng/L		-669.61	-100	10.31	ng/L	263.56	ng/L
	MeHg Unfiltered	2.64	ng/L		-2.64	-100	0.20	ng/L	1.13	ng/L
	HgT Unfiltered	699.18	ng/L		-699.18	-100	10.96	ng/L	275.32	ng/L
	Sediment									
	Hg0 porewater	26.93	ng/L		-26.93	-100	0.46	ng/L	10.629	ng/L
	HgII porewater	73.21	ng/L		-73.21	-100	1.10	ng/L	28.799	ng/L
	MeHg porewater	0.91	ng/L		-0.91	-100	0.04	ng/L	0.378	ng/L
	HgT porewater	101.06	ng/L		-101.06	-100	1.60	ng/L	39.806	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.26	ug/g		-33.26	-100	0.27	ug/g	13.08	ug/g
	MeHg bulk, dry	0.00827	ug/g	0.00422	0.00	-48.97966	0.00	ug/g	0.00	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.499	ug/g	13.09	ug/g
	Trophic Level 3	0.42	ug/g		-0.42	-100	0.064	ug/g	0.20	ug/g
	Trophic Level 4	0.91	ug/g		-0.91	-100	0.140	ug/g	0.44	ug/g
	HI	2.09					0.32		1.00	
	Sensitive Indicator	Great Blue Heron					Great Blue Heron		Great Blue Heron	
	Target C_sed, dry	13.09	ug/g	Note: 8						
	Target C_sed, wet	5.90	ug/g							

Rate Constants

Process	Media	Value	Units		
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		ratio Sed
1.00E-03	Sediment	1.16E-07	per day		Meth/demeth
Demethylation	Epilimnion	1.16E-08	per day		50.00%
1.00E-03	Hypolimnion	1.16E-07	per day		
2.00E-03	Sediment	2.33E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

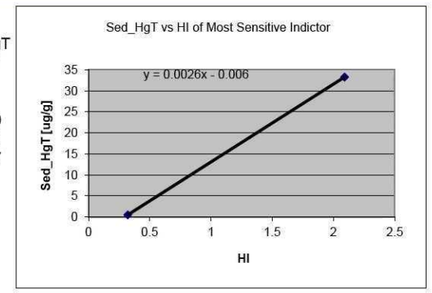
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.51	0.08	0.25
Otter	0.55	0.08	0.26
Mink	**1.07**	0.16	0.51
Great Blue Heron	**2.09**	0.32	**1.00**
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.98	0.15	0.47
Kingfisher	0.00	0.00	0.00
Wood Duck	0.38	0.06	0.18
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
2.09	33.27
0.32	0.50
m =	18.519
b=	-5.431
Sed_HgT	13.087
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.46	0.07	0.220	ng/L

Biota

Trophic Level 1: Phytoplankton	0.09	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Insects	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.42	0.06	0.20	ug Hg/ g wet weight
Trophic Level 4: Bass	0.91	0.14	0.44	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.50	0.08	0.24	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.09	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.04	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

Animal	Body Weight [kg in wet weight]	Ingestion Rate [kg wet weight/d]	Drinking rate [L/d]	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants --	Percent of Diet from Trophic Level 2 : Insects --	Percent of Diet from Trophic Level 2 : Crayfish or Frogs --	Percent of Diet from Trophic Level 3 : Fish --	Percent of Diet from Trophic Level 4 : Fish --	Percent of Diet from nonaquatic sources --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	39	0	0	0	39	75	0.51
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	31	9	41	75	0.55
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	74	81	75	**1.07**
Great Blue Heron	2.2	0.509	0.1	0%	5%	10%	50%	35%	0%	0	0	1	2	49	74	125	60	**2.09**
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	19	7	34	0	59	60	0.98
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	18	5	0	0	0	23	60	0.38
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	9	5000	0.00

Human

	Human Specific Parameters																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.011	0.00	5.91	0.00	0.00	0.00	6	75	0.08
0.006	0.00	0.00	0.19	4.78	1.39	6	75	0.08
0.007	0.00	0.00	0.60	0.43	11.32	12	75	0.16
0.003	0.00	0.14	0.29	7.44	11.34	19	60	0.32
0.033	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.005	0.00	2.84	1.02	5.18	0.00	9	60	0.15
0.008	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.005	2.72	0.80	0.00	0.00	0.00	4	60	0.06
0.000	0.00	0.00	0.07	0.17	1.07	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.035	0.00	18.45	0.00	0.00	0.00	18	75	0.25
0.018	0.00	0.00	0.59	14.92	4.33	20	75	0.26
0.022	0.00	0.00	1.87	1.35	35.35	39	75	0.51
0.010	0.00	0.42	0.92	23.24	35.42	60	60	**1.00**
0.103	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.016	0.00	8.87	3.19	16.19	0.00	28	60	0.47
0.025	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.015	8.49	2.50	0.00	0.00	0.00	11	60	0.18
0.000	0.00	0.00	0.22	0.55	3.35	4	5000	0.00
							RfD	
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Great Blue Heron

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Great Blue Heron

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893.2	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C Hg0 1 Aq			g/m3	4.73E-07	0.47
C HgII 1 Aq			g/m3	9.11E-08	0.09
C MeHg 1 Aq			g/m3	7.04E-08	0.07
C Hg0 2 Aq			g/m3	4.60E-07	0.46
C HgII 2 Aq			g/m3	1.65E-06	1.65
C MeHg 2 Aq			g/m3	1.79E-07	0.18
C Hg0 pore			g/m3	4.60E-07	0.46
C HgII pore			g/m3	1.10E-06	1.10
C MeHg pore			g/m3	4.38E-08	0.04
C HgT 1 filtered			g/m3	6.34E-07	0.63
C HgT 2 filtered			g/m3	2.29E-06	2.29
C HgT Sed filtered			g/m3	1.60E-06	1.60
C Hg0 1 T			g/m3	4.73E-07	0.47
C HgII 1 T			g/m3	2.69E-06	2.69
C MeHg 1 T			g/m3	1.36E-07	0.14
C Hg0 2 T			g/m3	4.60E-07	0.46
C HgII 2 T			g/m3	1.03E-05	10.31
C MeHg 2 T			g/m3	1.97E-07	0.20
C Hg0 sed, bulk			g/m3	3.82E-07	0
C HgII 1 sed, bulk			g/m3	2.25E-01	224,763
C MeHg 1 sed, bulk			g/m3	1.79E-04	179
C Hg0 sed, wet			g/g	2.98E-13	0.000
C HgII 1 sed, wet			g/g	2.69E-07	0.269
C MeHg 1 sed, wet			g/g	1.32E-14	0.000
C HgT sed,wet			g/g	2.69E-07	0.269
C Hg0 sed, dry weight			g/g	8.47E-13	0.0000
C HgII 1 sed, dry weight			g/g	4.99E-07	0.4989
C MeHg 1 sed, dry weight			g/g	3.96E-10	0.0004
C HgT 1			g/m3	3.30E-06	3.296
C HgT 2			g/m3	1.10E-05	10.964
C HgT Sed, dry weight			g/g	4.99E-07	0.499

	(%Me MeHg T/Hg T)	% MeHg	%HgII	% Hg0
Layer 1		4.14%	81.52%	14.34%
Layer 2		1.79%	94.01%	4.19%
Sediments		0.08%	99.92%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V 1	Volume of Layer 1	Aw*z 1	m3	648,711
V 2	Volume of Layer 2	Aw*z 2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10
f aq Hg0 w 1	aqueous phase fraction of Hg0 in water column, layer 1			1.000
f aq MeHg w 1	aqueous phase fraction of MeHg in water column, layer 1			0.087
f aq Hg0 w 2	aqueous phase fraction of Hg0 in water column, layer 2			1.000
f aq HgII w 2	aqueous phase fraction of HgII in water column, layer 2			0.028
f aq MeHg w 2	aqueous phase fraction of MeHg in water column, layer 2			0.153
f DOC Hg0 w 1	DOC complexed fraction of Hg0 in water column, layer 1			0.000
f DOC HgII w 1	DOC complexed fraction of HgII in water column, layer 1			0.028
f DOC MeHg w 1	DOC complexed fraction of MeHg in water column, layer 1			0.429
f DOC Hg0 w 2	DOC complexed fraction of Hg0 in water column, layer 2			0.000
f DOC HgII w 2	DOC complexed fraction of HgII in water column, layer 2			0.133
f DOC MeHg w 2	DOC complexed fraction of MeHg in water column, layer 2			0.757

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{o(Hg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{z1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{1B} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{o(HgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{z1} \cdot f^{w,1}_{abioHgII} A_w - v_{1B} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{o(MeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{z1} \cdot f^{w,1}_{abioMeHg} A_w - v_{1B} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{z1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{1B} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{z1} \cdot f^{w,2}_{abioHgII} A_w - v_{1B} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{z1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{1B} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{z1} \cdot f^{w,2}_{abioHg0} + v_{1B} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{z1} \cdot f^{w,2}_{abioHgII} + v_{1B} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{z1} \cdot f^{w,2}_{abioMeHg} + v_{1B} \cdot f^{w,2}_{bio,MeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	C Hg0 1 T	C HgII 1 T	C MeHg 1 T	C Hg0 2 T	C HgII 2 T	C MeHg 2 T	C Hg0 1 sed	C HgII 1 sed	C MeHg 1 sed
	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01
C HgII 1 T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-6.18E+01
C MeHg 1 T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	-1.43E+00
C Hg0 2 T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+08	0.00E+00	0.00E+00	-5.25E+03	1.18E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03

A*x=b

Matrix b

C Hg0 1 T	0.00E+00
C HgII 1 T	0.00E+00
C MeHg 1 T	0.00E+00
C Hg0 2 T	0.00E+00
C HgII 2 T	0.00E+00
C MeHg 2 T	0.00E+00
C Hg0 sed	0.00E+00
C HgII 1 sed	0.00E+00
C MeHg 1 sed	0.00E+00

Solution Matrix

C Hg0 1 T	4.728E-07
C HgII 1 T	2.687E-06
C MeHg 1 T	1.365E-07
C Hg0 2 T	4.599E-07
C HgII 2 T	1.031E-05
C MeHg 2 T	1.965E-07
C Hg0 sed	3.817E-07
C HgII 1 sed	2.248E-01
C MeHg 1 sed	1.785E-04

Inverted Matrix

-8.15E-09	-7.51E-09	-3.03E-09	-7.64E-09	-7.52E-09	-3.06E-09	-7.64E-09	-7.52E-09	-3.06E-09
-3.41E-08	-4.29E-08	-1.27E-08	-4.09E-08	-4.25E-08	-1.29E-08	-4.09E-08	-4.25E-08	-1.29E-08
-1.47E-10	-1.83E-10	-8.72E-08	-3.23E-10	-3.65E-10	-8.66E-08	-3.23E-10	-3.75E-10	-8.66E-08
-6.306E-09	-7.327E-09	-2.510E-09	-4.49E-08	-1.32E-08	-2.79E-09	-4.49E-08	-1.32E-08	-2.79E-09
-1.324E-07	-1.645E-07	-4.994E-08	-2.90E-07	-3.28E-07	-5.15E-08	-2.90E-07	-3.28E-07	-5.16E-08
-4.770E-10	-5.926E-10	-1.113E-07	-1.04E-09	-1.18E-09	-2.80E-07	-1.04E-09	-1.21E-09	-2.80E-07
-5.23E-09	-6.08E-09	-2.08E-09	-3.73E-08	-1.09E-08	-2.31E-09	-3.24E-06	-1.09E-08	-2.31E-09
-2.89E-03	-3.59E-03	-1.09E-03	-6.32E-03	-7.14E-03	-1.12E-03	-6.32E-03	-7.33E-03	-1.13E-03
-6.94E-07	-8.62E-07	-8.71E-05	-1.52E-06	-1.72E-06	-2.19E-04	-1.52E-06	-1.76E-06	-4.07E-04

x=b/A

4.72774E-07
2.68676E-06
1.36458E-07
4.59867E-07
1.03079E-05
1.96543E-07
3.8169E-07
0.224762892
0.000178549

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.006
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.039
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.093
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.744
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.123
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.037
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.800
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.090
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		4.06E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		2.04E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2]\left[H^+\right]^2}{[Hg^{2+}]} = 10^{-42}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} = \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS}$$
$$\frac{}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.61
C_HgII_1_Aq			g/m3	2.99E-06	2.99
C_MeHg_1_Aq			g/m3	4.59E-07	0.46
C_Hg0_2_Aq			g/m3	2.69E-05	26.93
C_HgII_2_Aq			g/m3	1.07E-04	107.30
C_MeHg_2_Aq			g/m3	2.40E-06	2.40
C_Hg0_pore			g/m3	2.69E-05	26.93
C_HgII_pore			g/m3	7.32E-05	73.21
C_MeHg_pore			g/m3	9.14E-07	0.91
C_HgT_1_filtered			g/m3	1.91E-05	19.07
C_HgT_2_filtered			g/m3	1.37E-04	136.63
C_HgT_Sed_filtered			g/m3	1.01E-04	101.06
C_Hg0_1_T			g/m3	1.56E-05	15.61
C_HgII_1_T			g/m3	8.83E-05	88.25
C_MeHg_1_T			g/m3	8.90E-07	0.89
C_Hg0_2_T			g/m3	2.69E-05	26.93
C_HgII_2_T			g/m3	6.70E-04	669.61
C_MeHg_2_T			g/m3	2.64E-06	2.64
C_Hg0_sed			g/m3	2.24E-05	22.35
C_HgII_1_sed			g/m3	1.50E+01	14984386.47
C_MeHg_1_sed			g/m3	3.73E-03	3726.18
C_Hg0_sed, wet			g/g	8.44E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.702
C_MeHg_1_sed, wet			g/g	4.46E-09	0.004
C_HgT_sed,wet			g/g	1.17E-05	11.706
C_Hg0_sed, dry weight			g/g	4.96E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.33E-05	33.26
C_MeHg_1_sed, dry weight			g/g	8.27E-09	0.01
C_HgT_1			g/m3	1.05E-04	104.75
C_HgT_2			g/m3	6.99E-04	699.18
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		0.85%	84.25%	14.90%
Layer 2			0.38%	95.77%	3.85%
Sediments			0.02%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.58263%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.65526%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	2.75205%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	2.80992%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	42.93010%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	13.27265%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.04824%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photord} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{methg} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{methg} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorMe} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorMe} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{methg} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{methg2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorMe} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix										x=b/A
C_Hg0_1_T	1.561E-05	-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	1.56E-05
C_HgII_1_T	8.825E-05	-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	8.83E-05
C_MeHg_1_T	8.905E-07	-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-15	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	8.9E-07
C_Hg0_2_T	2.693E-05	-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	2.69E-05
C_HgII_2_T	6.696E-04	-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.00067
C_MeHg_2_T	2.635E-06	-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	2.64E-06
C_Hg0_sed	2.235E-05	-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	2.24E-05
C_HgII_1_sed	1.498E+01	9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	14.98439
C_MeHg_1_sed	3.726E-03	-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.003726

A*x=b

C_T_sed 14.988135 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	564.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq\_i}^{sw,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

v_sA	abiotic settling velocity		m/yr	4792.628412
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	13900.95
TSS_1			mg/L	1.80
TSS+2			mg/L	0.43

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

Effective Partition Coefficients for each Hg species and layer

K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for HgII in layer 1	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for HgII in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	6.29E-06	6.29
C_HgII_1_Aq			g/m3	1.21E-06	1.21
C_MeHg_1_Aq			g/m3	2.20E-07	0.22
C_Hg0_2_Aq			g/m3	1.06E-05	10.63
C_HgII_2_Aq			g/m3	4.22E-05	42.23
C_MeHg_2_Aq			g/m3	1.03E-06	1.03
C_Hg0_pore			g/m3	1.06E-05	10.63
C_HgII_pore			g/m3	2.88E-05	28.80
C_MeHg_pore			g/m3	3.78E-07	0.38
C_HgT_1_filtered			g/m3	7.71E-06	7.71
C_HgT_2_filtered			g/m3	5.39E-05	53.89
C_HgT_Sed_filtered			g/m3	3.98E-05	39.81
C_Hg0_1_T			g/m3	6.29E-06	6.29
C_HgII_1_T			g/m3	3.56E-05	35.55
C_MeHg_1_T			g/m3	4.26E-07	0.43
C_Hg0_2_T			g/m3	1.06E-05	10.63
C_HgII_2_T			g/m3	2.64E-04	263.56
C_MeHg_2_T			g/m3	1.13E-06	1.13
C_Hg0_sed			g/m3	8.82E-06	8.82
C_HgII_1_sed			g/m3	5.89E+00	5,894,221.02
C_MeHg_1_sed			g/m3	1.54E-03	1,541.26
C_Hg0_sed, wet			g/g	3.33E-12	0.00
C_HgII_1_sed, wet			g/g	4.60E-06	4.60
C_MeHg_1_sed, wet			g/g	1.85E-09	0.00
C_HgT_sed,wet			g/g	4.60E-06	4.60
C_Hg0_sed, dry weight			g/g	1.96E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.31E-05	13.08
C_MeHg_1_sed, dry weight			g/g	3.42E-09	0.00
C_HgT_1			g/m3	4.23E-05	42.27
C_HgT_2			g/m3	2.75E-04	275.32
C_HgT_Sed, dry weight			g/g	1.31E-05	13.09
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		1.01%	84.11%	14.88%
Layer 2			0.41%	95.73%	3.86%
Sediments			0.03%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.58263%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.65526%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	2.75205%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	2.80992%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	42.93010%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	13.27265%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	75.71189%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{Hg1l1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{Hg1l}}{dt} = L_{T,Hg1l} + Q_{in}C_{in,Hg1l} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHg1l} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abiaHg1l} A_w - v_{sB} \cdot f^{w,1}_{bioHg1l} A_w\right] \cdot C^w_{Hg1l} + Q' \cdot C^w_{Hg1l}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{Hg1l} + \left[-Q_{out} - Q' - kw_{oIMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abiMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{Hg1l2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abiHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{Hg1l2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abiaHg1l} A_w - v_{sB} \cdot f^{w,2}_{bioHg1l} A_w - R_{sw} \cdot f^{w,2}_{aqHg1l}\right] \cdot C^w_{Hg1l2} + Q' \cdot C^w_{Hg1l} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg1l}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg1l} A_w\right] \cdot C^{sed}_{aqHg1l}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{Hg1l2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abiaMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioaMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aq,Hg0} + \left(v_{s1} \cdot f^{w,2}_{abiaHg0} + v_{sB} \cdot f^{w,2}_{bio,Hg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,Hg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{Hg1l} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{Hg1l}}{dt} = \left[R_{sw} f^{w,2}_{aqHg1l} + \left(v_{s1} \cdot f^{w,2}_{abiaHg1l} + v_{sB} \cdot f^{w,2}_{bioHg1l}\right) \cdot A_w\right] \cdot C^w_{Hg1l} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg1l}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,Hg1l} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{Hg1l} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abiaMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{Hg1l} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,MeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed
	1	2	3	4	5	6	7	8	9
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03

Matrix b	
C_Hg0_1_T	-4.89E-01
C_HgII_1_T	-6.18E+01
C_MeHg_1_T	-1.43E+00
C_Hg0_2_T	0.00E+00
C_HgII_2_T	0.00E+00
C_MeHg_2_T	0.00E+00
C_Hg0_sed	0.00E+00
C_HgII_1_sed	5.90E+00
C_MeHg_1_sed	0.00E+00

Target C_sed, wet 5.895771109 g/g

Solution Matrix	
C_Hg0_1_T	6.288E-06
C_HgII_1_T	3.555E-05
C_MeHg_1_T	4.261E-07
C_Hg0_2_T	1.063E-05
C_HgII_2_T	2.636E-04
C_MeHg_2_T	1.133E-06
C_Hg0_sed	8.822E-06
C_HgII_1_sed	5.894E+00
C_MeHg_1_sed	1.541E-03

Inverted Matrix										x=b/A
-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	6.29E-06	
-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	3.56E-05	
-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-16	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	4.26E-07	
-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	1.06E-05	
-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.000264	
-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	1.13E-06	
9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	5.894221	
-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.001541	

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate cc	per yr	134.70
kw_v,HgII	water column volatilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatilization loss rate cc	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	122.63
kw_red_2	water column reduction rate constant,	per yr	23.27
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for l	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for l	per yr	0.82
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.153 \text{6x} 10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \Big/ \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{C_{filtered,i}^j}{C_{diss,i}^j + C_{DOC,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = (D_{dry,i} + D_{wet,i}) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.58263%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75205%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.65526%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.80992%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			13.27265%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			42.93010%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.56114%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			3.93251%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01844%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.29998%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			74.39982%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.34651%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			80.04279%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			3.70796%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.97965%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.17
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.23
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	1,430.88
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3			
Sbio_phyto,1	1	TSS_1	1.80	mg/L
Sbio_zoo,1	0.5	TSS_2	0.43	mg/L
Sbio_phyto,2	0			
Sbio_zoo,2	0			
Sabio_1	1.34E-01			
Sabio_2	1.99E-01			
Sbio_dead,1	1.66E-01			
Sbio_dead,2	2.28E-01			
S_abio, sed	8.42E+04			
S_bio_dead,sed	1.43E+03			
S_sed,total	8.57E+04	g/m3		

Matrix A

	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed
	1	2	3	4	5	6
S_abio,1	2.22E+09	5.86E+06	0	0	0	0
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03

b

S_abio,1	2.99E+08
S_abio,2	0
S_bio_dead,1	7.10E+06
S_bio_dead,2	0
S_abio,sed	0
S_bio_dead,sed	0

Solution Matrix

S_abio,1	1.34E-01
S_abio,2	1.99E-01
S_bio_dead,1	1.66E-01
S_bio_dead,2	2.28E-01
S_abio,sed	8.42E+04
S_bio_dead,sed	1.43E+03

Matrix Inversion

						x=b/A
4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
0	0	2.34E-08	4.73E-09	0	1.51E-09	0.165948
0	0	3.21E-08	-2.81E-08	0	-8.94E-09	0.227765
0	0	0	0	-2.82E-04	0	84224.58
0.000282	-2.81E-04	0	0	0	0	1430.879
0	0	0.000201	-1.76E-04	0	-2.42E-04	

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

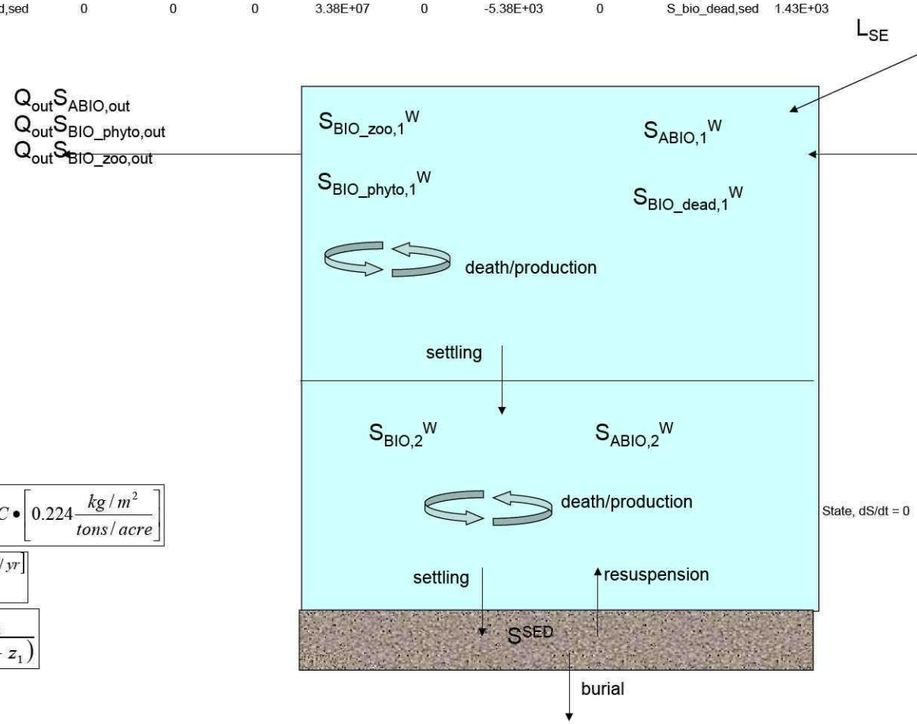
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS_{abio,1}^{w}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S_{abio,1}^{w} - v_{sA} \cdot A_w \cdot S_{abio,1}^{w}$$

$$V_2 \frac{dS_{abio,2}^{w}}{dt} = +v_{sA} \cdot A_w \cdot S_{abio,1}^{w} - v_{sA} \cdot A_w \cdot S_{abio,2}^{w} + v_{rs} \cdot A_w \cdot S_{abio}^{sed}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankton (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

5	Modeled from Wetzel			
	Wetzel (mg C/m2/day)	50-300	250-1000	>1000	<50-500
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abiq2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00583	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.02752		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.02810		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.13273		
k_meth_1	abiotic methylation in layer 1		per yr	2.47E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	6.81E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			5.83E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.81E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.33E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	1.44E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	6.81E-06	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	1
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

$$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$$

1 UV-B is modeled as being 0.5% of visible light.
check?

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43* ,135.

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Pied-Billed Grebe

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	-29.48965936
MeHg	7.33E-08	g/m3	0.07332	31.2197083

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27	ug/g	
Known Mercury in Contaminated Soils			
Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	
Required Hazard Index for Sensitive Indicator	1		

Kd_abio			
HgII	7,182,936	1	
MeHg	15,887	1	
Kd_bio			
HgII	127,696,640	1	
MeHg	2,581,565	1	
Kd_DOC			
HgII	301,427	1	
MeHg	310,000	1	
	PCT ERROR	CLEANUP	
MeHg Filtered	3.46	33.90	
HgT Filtered	-61.23		
MeHg Unfilter	-0.92		
HgT Unfiltere	-59.26		

Exposure Concentrations

		Scenario 1 With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2 Background Conditions		Scenario 3 Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.61	ng/L		-15.61	-100	0.47	ng/L	15.91	ng/L
	HgII Filtered	2.99	ng/L		-2.99	-100	0.09	ng/L	3.05	ng/L
Epilimnion	MeHg Filtered	0.46	ng/L	0.47525	0.02	3.4600979	0.07	ng/L	0.47	ng/L
	HgT Filtered	19.07	ng/L	7.39	-11.68	-61.23396	0.63	ng/L	19.42	ng/L
	Hg0 Unfiltered	15.61	ng/L		-15.61	-100	0.47	ng/L	15.91	ng/L
	HgII Unfiltered	88.25	ng/L		-88.25	-100	2.69	ng/L	89.90	ng/L
	MeHg Unfiltered	0.89	ng/L	0.88225	-0.01	-0.923906	0.14	ng/L	0.91	ng/L
	HgT Unfiltered	104.75	ng/L	42.67625	-62.08	-59.26087	3.30	ng/L	106.71	ng/L
Hypolimnion	Hg0 Filtered	26.93	ng/L		-26.93	-100	0.46	ng/L	27.44	ng/L
	HgII Filtered	107.30	ng/L		-107.30	-100	1.65	ng/L	109.34	ng/L
	MeHg Filtered	2.40	ng/L		-2.40	-100	0.18	ng/L	2.44	ng/L
	HgT Filtered	136.63	ng/L		-136.63	-100	2.29	ng/L	139.23	ng/L
	Hg0 Unfiltered	26.93	ng/L		-26.93	-100	0.46	ng/L	27.44	ng/L
	HgII Unfiltered	669.61	ng/L		-669.61	-100	10.31	ng/L	682.33	ng/L
	MeHg Unfiltered	2.64	ng/L		-2.64	-100	0.20	ng/L	2.68	ng/L
	HgT Unfiltered	699.18	ng/L		-699.18	-100	10.96	ng/L	712.46	ng/L
	Sediment									
	Hg0 porewater	26.93	ng/L		-26.93	-100	0.46	ng/L	27.443	ng/L
	HgII porewater	73.21	ng/L		-73.21	-100	1.10	ng/L	74.606	ng/L
	MeHg porewater	0.91	ng/L		-0.91	-100	0.04	ng/L	0.930	ng/L
	HgT porewater	101.06	ng/L		-101.06	-100	1.60	ng/L	102.980	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.26	ug/g		-33.26	-100	0.27	ug/g	33.89	ug/g
	MeHg bulk, dry	0.00827	ug/g	0.00422	0.00	-48.97966	0.00	ug/g	0.01	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.499	ug/g	33.90	ug/g
Fish	Trophic Level 3	0.42	ug/g		-0.42	-100	0.064	ug/g	0.43	ug/g
	Trophic Level 4	0.91	ug/g		-0.91	-100	0.140	ug/g	0.93	ug/g
	HI	0.98					0.15		1.00	
	Sensitive Indicator	Pied-bill Grebe					Pied-bill Grebe		Pied-bill Grebe	
	Target C_sed, dry	33.90	ug/g	Note: 8						
	Target C_sed, wet	15.27	ug/g							

Rate Constants

Process		Media	Value	Units		
Methylation		Epilimnion	1.16E-07	per day	1.16E-04	
		Hypolimnion	1.16E-06	per day		ratio Sed
	1.00E-03	Sediment	1.16E-07	per day		Meth/demeth
Demethylation		Epilimnion	1.16E-08	per day		50.00%
	1.00E-03	Hypolimnion	1.16E-07	per day		
	2.00E-03	Sediment	2.33E-07	per day		
Biotic Reduction		Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)		Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light		Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B		Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B		Water Column	58.85	per day per E/m2-day		
Dark Oxidation		Water Column	1.44	per day		

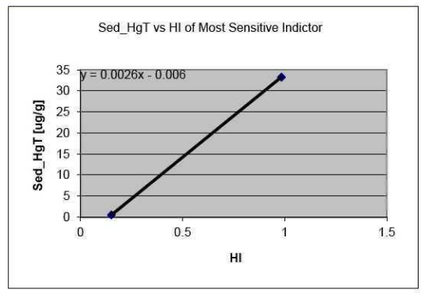
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.51	0.08	0.52
Otter	0.55	0.08	0.56
Mink	0.00	0.00	0.00
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.98	0.15	**1.00**
Kingfisher	0.00	0.00	0.00
Wood Duck	0.38	0.06	0.39
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
0.98	33.27
0.15	0.50
m =	39.334
b=	-5.431
Sed_HgT	33.902
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.

Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

	Site-Specific User Input	Required
	Model Calculated	No input required
	Data Necessary for certain sites	Only necessary if applicable to site of interest
	Scenario 1 Output	
	Scenario 2 Output	
	Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

	Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]		0.46	0.07	0.467	ng/L

Biota

Trophic Level 1: Phytoplankton		0.09	0.01	0.09	ug Hg/ g wet weight
Trophic Level 2: Insects		0.08	0.01	0.08	ug Hg/ g wet weight
Trophic Level 2: Crayfish		0.08	0.01	0.08	ug Hg/ g wet weight
Trophic Level 3 : Bluegill		0.42	0.06	0.43	ug Hg/ g wet weight
Trophic Level 4: Bass		0.91	0.14	0.93	ug Hg/ g wet weight
Trophic Level 3: Silverside		0.50	0.08	0.50	ug Hg/ g wet weight
Trophic Level: 3 Crayfish		0.09	0.01	0.09	ug Hg/ g wet weight
Trophic Level 3: Bullfrog		0.08	0.01	0.08	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Body Weight	Ingestion Rate	Drinking rate	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants	Percent of Diet from Trophic Level 2 : Insects	Percent of Diet from Trophic Level 2 : Crayfish or Frogs	Percent of Diet from Trophic Level 3 : Fish	Percent of Diet from Trophic Level 4 : Fish	Percent of Diet from nonaquatic sources	Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Insects	Potential Dose from Trophic Level 2: Crayfish	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
Animal	[kg in wet weight]	[kg wet weight/d]	[L/d]	--	--	--	--	--	--	[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	39	0	0	0	39	75	0.51
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	31	9	41	75	0.55
Mink	0.85	0.1145	0.085	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	75	0.00
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	19	7	34	0	59	60	0.98
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	18	5	0	0	0	23	60	0.38
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	9	5000	0.00
Human																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.011	0.00	5.91	0.00	0.00	0.00	6	75	0.08
0.006	0.00	0.00	0.19	4.78	1.39	6	75	0.08
0.007	0.00	0.00	0.00	0.00	0.00	0	75	0.00
0.003	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.033	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.005	0.00	2.84	1.02	5.18	0.00	9	60	0.15
0.008	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.005	2.72	0.80	0.00	0.00	0.00	4	60	0.06
0.000	0.00	0.00	0.07	0.17	1.07	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.075	0.00	39.19	0.00	0.00	0.00	39	75	0.52
0.039	0.00	0.00	1.25	31.70	9.20	42	75	0.56
0.047	0.00	0.00	0.00	0.00	0.00	0	75	0.00
0.021	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.220	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.034	0.00	18.85	6.77	34.38	0.00	60	60	**1.00**
0.053	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.031	18.03	5.31	0.00	0.00	0.00	23	60	0.39
0.000	0.00	0.00	0.47	1.16	7.12	9	5000	0.00
							RfD	
0.008	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Pied-Billed Grebe

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Pied-Billed Grebe

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Coun	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeHg	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Pied-Billed Grebe

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and reflec		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

this table does not all correspond to EPA Report to Congress - check!

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	
HgII	Mean	58,000	50000	100,000	200,000	
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000		
MeHg	Mean	7000	3000	100,000	500,000	
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000		
Hg0		1,000	1,000	3000	1,000	NTG added these 11/1/19

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.73E-07	0.47
C_HgII_1_Aq			g/m3	9.11E-08	0.09
C_MeHg_1_Aq			g/m3	7.04E-08	0.07
C_Hg0_2_Aq			g/m3	4.60E-07	0.46
C_HgII_2_Aq			g/m3	1.65E-06	1.65
C_MeHg_2_Aq			g/m3	1.79E-07	0.18
C_Hg0_pore			g/m3	4.60E-07	0.46
C_HgII_pore			g/m3	1.10E-06	1.10
C_MeHg_pore			g/m3	4.38E-08	0.04
C_HgT_1_filtered			g/m3	6.34E-07	0.63
C_HgT_2_filtered			g/m3	2.29E-06	2.29
C_HgT_Sed_filtered			g/m3	1.60E-06	1.60
C_Hg0_1_T			g/m3	4.73E-07	0.47
C_HgII_1_T			g/m3	2.69E-06	2.69
C_MeHg_1_T			g/m3	1.36E-07	0.14
C_Hg0_2_T			g/m3	4.60E-07	0.46
C_HgII_2_T			g/m3	1.03E-05	10.31
C_MeHg_2_T			g/m3	1.97E-07	0.20
C_Hg0_sed, bulk			g/m3	3.82E-07	0
C_HgII_1_sed, bulk			g/m3	2.25E-01	224,763
C_MeHg_1_sed, bulk			g/m3	1.79E-04	179
C_Hg0_sed, wet			g/g	2.98E-13	0.000
C_HgII_1_sed, wet			g/g	2.69E-07	0.269
C_MeHg_1_sed, wet			g/g	1.32E-14	0.000
C_HgT_sed,wet			g/g	2.69E-07	0.269
C_Hg0_sed, dry weight			g/g	8.47E-13	0.0000
C_HgII_1_sed, dry weight			g/g	4.99E-07	0.4989
C_MeHg_1_sed, dry weight			g/g	3.96E-10	0.0004
C_HgT_1			g/m3	3.30E-06	3.296
C_HgT_2			g/m3	1.10E-05	10.964
C_HgT_Sed, dry weight			g/g	4.99E-07	0.499

			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		4.14%	81.52%	14.34%
Layer 2			1.79%	94.01%	4.19%
Sediments			0.08%	99.92%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V_1	Volume of Layer 1	Aw*z_1	m3	648,711
V_2	Volume of Layer 2	Aw*z_2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.006
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.087
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.028
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.153
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.028
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.429
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.133
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.757

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored1} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth,2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+08	0.00E+00	0.00E+00	-5.25E+03	1.18E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03

b

C Hg0 1 T	-4.89E-01
C HgII 1 T	-6.18E+01
C MeHg 1 T	-1.43E+00
C Hg0 2 T	5.25E+03
C HgII 2 T	0.00E+00
C MeHg 2 T	5.30E+03
C Hg0 sed	0.00E+00
C HgII 1 sed	-5.25E+03
C MeHg 1 sed	1.18E+00

A*x=b

Matrix

C Hg0 1 T	4.728E-07
C HgII 1 T	2.687E-06
C MeHg 1 T	1.365E-07
C Hg0 2 T	4.599E-07
C HgII 2 T	1.031E-05
C MeHg 2 T	1.965E-07
C Hg0 sed	3.817E-07
C HgII 1 sed	2.248E-01
C MeHg 1 sed	1.785E-04

Solution

Inverted Matrix

C Hg0 1 T	-8.15E-09	-7.51E-09	-3.03E-09	-7.64E-09	-7.52E-09	-3.06E-09	-7.64E-09	-7.52E-09	-3.06E-09
C HgII 1 T	-3.41E-08	-4.29E-08	-1.27E-08	-4.09E-08	-4.25E-08	-1.29E-08	-4.09E-08	-4.25E-08	-1.29E-08
C MeHg 1 T	-1.47E-10	-1.83E-10	-8.72E-08	-3.23E-10	-3.65E-10	-8.66E-08	-3.23E-10	-3.75E-10	-8.66E-08
C Hg0 2 T	-6.306E-09	-7.327E-09	-2.510E-09	-4.49E-08	-1.32E-08	-2.79E-09	-4.49E-08	-1.32E-08	-2.79E-09
C HgII 2 T	-1.324E-07	-1.645E-07	-4.994E-08	-2.90E-07	-3.28E-07	-5.15E-08	-2.90E-07	-3.28E-07	-5.16E-08
C MeHg 2 T	-4.770E-10	-5.926E-10	-1.113E-07	-1.04E-09	-1.18E-09	-2.80E-07	-1.04E-09	-1.21E-09	-2.80E-07
C Hg0 sed	-5.23E-09	-6.08E-09	-2.08E-09	-3.73E-08	-1.09E-08	-2.31E-09	-3.24E-06	-1.09E-08	-2.31E-09
C HgII 1 sed	-2.89E-03	-3.59E-03	-1.09E-03	-6.32E-03	-7.14E-03	-1.12E-03	-6.32E-03	-7.33E-03	-1.13E-03
C MeHg 1 sed	-6.94E-07	-8.62E-07	-8.71E-05	-1.52E-06	-1.72E-06	-2.19E-04	-1.52E-06	-1.76E-06	-4.07E-04

x=b/A

C Hg0 1 T	4.72774E-07
C HgII 1 T	2.68676E-06
C MeHg 1 T	1.36459E-07
C Hg0 2 T	4.59867E-07
C HgII 2 T	1.03079E-05
C MeHg 2 T	1.96543E-07
C Hg0 sed	3.8169E-07
C HgII 1 sed	0.224762892
C MeHg 1 sed	0.000178549

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.006
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			0.039
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			0.093
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			0.223
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			0.744
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			0.223
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			0.123
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			0.037
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			0.800
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			0.090
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			4.06E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			2.04E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			1.00E+00
L_T,Hg0	Total Load, Hg0		g/yr	4.89E-01
L_T,HgII	Total Load, HgII		g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg		g/yr	9.36E-01
Rate Constants				
kw_v,Hg0	water column volatilization loss rate constant, Hg0		per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII		per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg		per yr	0.63
kw_oxid_1	water column oxidation rate constant		per yr	554.95
kw_oxid_2	water column oxidation rate constant		per yr	525.60
kw_red_1	water column reduction rate constant, layer 2		per yr	122.63
kw_red_2	water column reduction rate constant, layer 2		per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1		per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2		per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1		per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2		per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1		per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2		per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant		per yr	0.00
kb_oxid	benthic oxidation rate constant		per yr	0.00
kb_red	benthic reduction rate constant		per yr	0.00
kb_methy	benthic methylation rate constant		per yr	0.00
kb_demeth	benthic demethylation rate constant		per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant		per yr	0.00
v_sA	abiotic settling velocity		m/yr	4,792.63
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.030
V_sed	Volume of Sediment	Aw*z_sed	m3	13900.95
TSS_1			mg/L	1.80
TSS+2			mg/L	0.43
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1		L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2		L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2		L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	2.32E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}}}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.61
C_HgII_1_Aq			g/m3	2.99E-06	2.99
C_MeHg_1_Aq			g/m3	4.59E-07	0.46
C_Hg0_2_Aq			g/m3	2.69E-05	26.93
C_HgII_2_Aq			g/m3	1.07E-04	107.30
C_MeHg_2_Aq			g/m3	2.40E-06	2.40
C_Hg0_pore			g/m3	2.69E-05	26.93
C_HgII_pore			g/m3	7.32E-05	73.21
C_MeHg_pore			g/m3	9.14E-07	0.91
C_HgT_1_filtered			g/m3	1.91E-05	19.07
C_HgT_2_filtered			g/m3	1.37E-04	136.63
C_HgT_Sed_filtered			g/m3	1.01E-04	101.06
C_Hg0_1_T			g/m3	1.56E-05	15.61
C_HgII_1_T			g/m3	8.83E-05	88.25
C_MeHg_1_T			g/m3	8.90E-07	0.89
C_Hg0_2_T			g/m3	2.69E-05	26.93
C_HgII_2_T			g/m3	6.70E-04	669.61
C_MeHg_2_T			g/m3	2.64E-06	2.64
C_Hg0_sed			g/m3	2.24E-05	22.35
C_HgII_1_sed			g/m3	1.50E+01	14984386.47
C_MeHg_1_sed			g/m3	3.73E-03	3726.18
C_Hg0_sed, wet			g/g	8.44E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.702
C_MeHg_1_sed, wet			g/g	4.46E-09	0.004
C_HgT_sed,wet			g/g	1.17E-05	11.706
C_Hg0_sed, dry weight			g/g	4.96E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.33E-05	33.26
C_MeHg_1_sed, dry weight			g/g	8.27E-09	0.01
C_HgT_1			g/m3	1.05E-04	104.75
C_HgT_2			g/m3	6.99E-04	699.18
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		0.85%	84.25%	14.90%
Layer 2			0.38%	95.77%	3.85%
Sediments			0.02%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.58263%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.65526%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	2.75205%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	2.80992%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	42.93010%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	13.27265%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.04824%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sed4Hg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed	Matrix b		Solution Matrix	Inverted Matrix									x=b/A	
	1	2	3	4	5	6	7	8	9														
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	1.561E-05	-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	1.56E-05	
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	8.825E-05	-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	8.83E-05	
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T	8.905E-07	-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-16	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	8.9E-07	
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	2.693E-05	-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	2.69E-05	
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	6.696E-04	-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.00067	
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T	2.635E-06	-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	2.64E-06	
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	2.235E-05	-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	2.24E-05	
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed	1.498E+01	9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	14.98439	
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed	3.726E-03	-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.003726	

C_T_sed 14.988135 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for HgII in layer 1	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for HgII in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \times 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{ioo}^{j} C_{ioo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{ioo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.59E-05	15.91
C_HgII_1_Aq			g/m3	3.05E-06	3.05
C_MeHg_1_Aq			g/m3	4.67E-07	0.47
C_Hg0_2_Aq			g/m3	2.74E-05	27.44
C_HgII_2_Aq			g/m3	1.09E-04	109.34
C_MeHg_2_Aq			g/m3	2.44E-06	2.44
C_Hg0_pore			g/m3	2.74E-05	27.44
C_HgII_pore			g/m3	7.46E-05	74.61
C_MeHg_pore			g/m3	9.30E-07	0.93
C_HgT_1_filtered			g/m3	1.94E-05	19.42
C_HgT_2_filtered			g/m3	1.39E-04	139.23
C_HgT_Sed_filtered			g/m3	1.03E-04	102.98
C_Hg0_1_T			g/m3	1.59E-05	15.91
C_HgII_1_T			g/m3	8.99E-05	89.90
C_MeHg_1_T			g/m3	9.05E-07	0.91
C_Hg0_2_T			g/m3	2.74E-05	27.44
C_HgII_2_T			g/m3	6.82E-04	682.33
C_MeHg_2_T			g/m3	2.68E-06	2.68
C_Hg0_sed			g/m3	2.28E-05	22.78
C_HgII_1_sed			g/m3	1.53E+01	15,269,157.31
C_MeHg_1_sed			g/m3	3.79E-03	3,794.63
C_Hg0_sed, wet			g/g	8.60E-12	0.00
C_HgII_1_sed, wet			g/g	1.19E-05	11.92
C_MeHg_1_sed, wet			g/g	4.54E-09	0.00
C_HgT_sed,wet			g/g	1.19E-05	11.93
C_Hg0_sed, dry weight			g/g	5.06E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.39E-05	33.89
C_MeHg_1_sed, dry weight			g/g	8.42E-09	0.01
C_HgT_1			g/m3	1.07E-04	106.71
C_HgT_2			g/m3	7.12E-04	712.46
C_HgT_Sed, dry weight			g/g	3.39E-05	33.90
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		0.85%	84.25%	14.90%
Layer 2			0.38%	95.77%	3.85%
Sediments			0.02%	99.98%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.58263%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.65526%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	2.75205%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	2.80992%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	42.93010%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	13.27265%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	75.71189%

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorel} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{biaHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHgII} A_w - v_{sB} \cdot f^{w,1}_{biaHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{oIMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorel} V_w - v_{sA} \cdot f^{w,1}_{abiaMeHg} A_w - v_{sB} \cdot f^{w,1}_{biaMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photorel} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{biaHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiaHgII} A_w - v_{sB} \cdot f^{w,2}_{biaHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorel} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiaMeHg} A_w - v_{sB} \cdot f^{w,2}_{biaMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abiaHg0} + v_{sB} \cdot f^{w,2}_{biaHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abiaHgII} + v_{sB} \cdot f^{w,2}_{biaHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abiaMeHg} + v_{sB} \cdot f^{w,2}_{biaMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	1.591E-05	-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	1.59E-05
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	8.990E-05	-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	8.99E-05
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T	9.050E-07	-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-16	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	9.05E-07
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	2.744E-05	-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	2.74E-05
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	6.823E-04	-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.000682
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T	2.683E-06	-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	2.68E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	2.278E-05	-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	2.28E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.53E+01	C_HgII_1_sed	1.527E+01	9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	15.26916
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed	3.795E-03	-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.003795

Target C_sed, wet 15.27297472 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate cc	per yr	134.70
kw_v,HgII	water column volatilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatilization loss rate cc	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	122.63
kw_red_2	water column reduction rate constant,	per yr	23.27
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for l	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for l	per yr	0.82
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{ag,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2]\left[H^+\right]^2}{\left[Hg^{2+}\right]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \Big/ \frac{C_{diss,i}^j + C_{DOC,i}^j}{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)} = \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} \Big/ \frac{C_{filtered,i}^j}{}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = (D_{dry,i} + D_{wet,i}) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.58263%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75205%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.65526%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.80992%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			13.27265%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			42.93010%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.56114%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			3.93251%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01844%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.29998%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			74.39982%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.34651%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			80.04279%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			3.70796%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.97965%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.17
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.23
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	1,430.88
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1	TSS_1	1.80	mg/L	
Sbio_zoo,1	0.5	TSS_2	0.43	mg/L	
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	1.66E-01				
Sbio_dead,2	2.28E-01				
S_abio, sed	8.42E+04				
S_bio_dead,sed	1.43E+03				
S_sed,total	8.57E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed									
	1	2	3	4	5	6	b		Matrix						x=b/A
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	7.10E+06	S_bio_dead,1	1.66E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.165948
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	2.28E-01	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	0.227765
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	1.43E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	1430.879

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

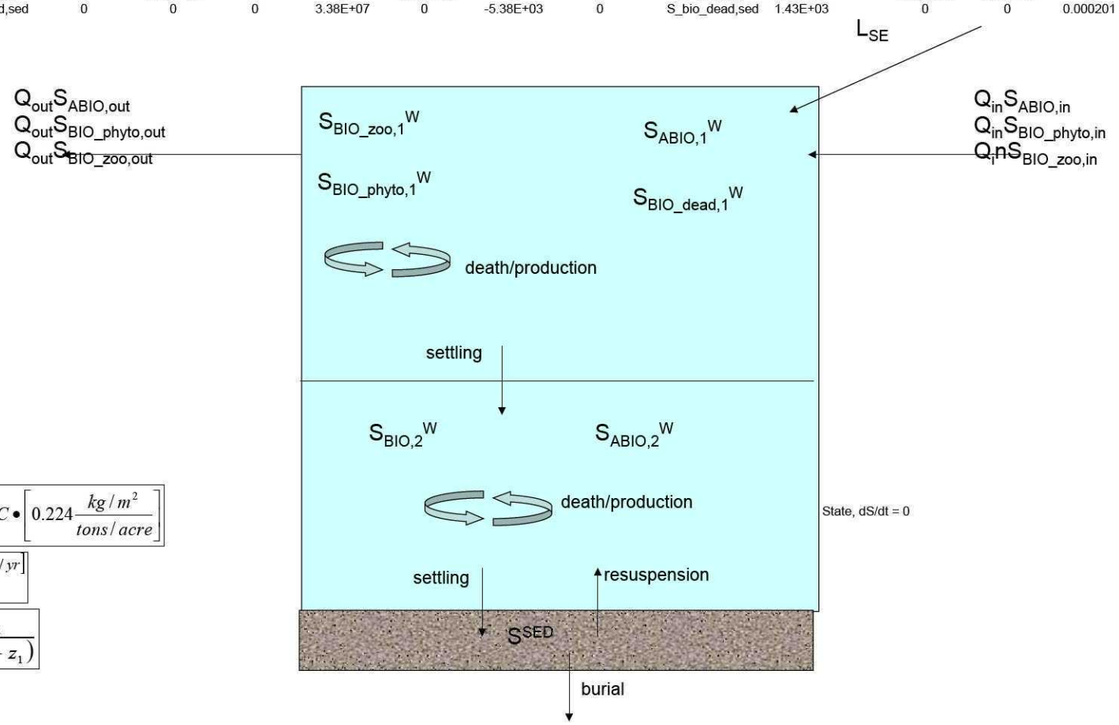
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Pied-Billed Grebe

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00583	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.02752		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.02810		$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.13273		
k_meth_1	abiotic methylation in layer 1		per yr	2.47E-07		$k_{meth} = k_{meth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC}\right)$
k_meth_2	abiotic* methylation in layer 2		per yr	6.81E-06	if anoxic:	

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1	
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07		
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06		
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			5.83E-03		
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75E-02		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.81E-02		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.33E-01		
k_demeth_1	biotic demethylation in layer 1		per yr	1.44E-07		$k_{demeth} = k_{demeth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC}\right)$
k_demeth_2	biotic demethylation in layer 2		per yr	6.81E-06		

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{1.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location	
East	YES
West	NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Mink

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	-29.48965936
MeHg	7.33E-08	g/m3	0.07332	31.2197083

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27	ug/g	

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio			
HgII	7,182,936	1	
MeHg	15,887	1	
Kd_bio			
HgII	127,696,640	1	
MeHg	2,581,565	1	
Kd_DOC			
HgII	301,427	1	
MeHg	310,000	1	
	PCT ERROR	CLEANUP	
MeHg Filtered	3.46	30.58	
HgT Filtered	-61.23		
MeHg Unfilter	-0.92		
HgT Unfiltere	-59.26		

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.61	ng/L		-15.61	-100	0.47	ng/L	14.37	ng/L
	HgII Filtered	2.99	ng/L		-2.99	-100	0.09	ng/L	2.76	ng/L
Epilimnion	MeHg Filtered	0.46	ng/L	0.47525	0.02	3.4600979	0.07	ng/L	0.43	ng/L
	HgT Filtered	19.07	ng/L	7.39	-11.68	-61.23396	0.63	ng/L	17.55	ng/L
	Hg0 Unfiltered	15.61	ng/L		-15.61	-100	0.47	ng/L	14.37	ng/L
	HgII Unfiltered	88.25	ng/L		-88.25	-100	2.69	ng/L	81.22	ng/L
	MeHg Unfiltered	0.89	ng/L	0.88225	-0.01	-0.923906	0.14	ng/L	0.83	ng/L
	HgT Unfiltered	104.75	ng/L	42.67625	-62.08	-59.26087	3.30	ng/L	96.42	ng/L
Hypolimnion	Hg0 Filtered	26.93	ng/L		-26.93	-100	0.46	ng/L	24.76	ng/L
	HgII Filtered	107.30	ng/L		-107.30	-100	1.65	ng/L	98.62	ng/L
	MeHg Filtered	2.40	ng/L		-2.40	-100	0.18	ng/L	2.22	ng/L
	HgT Filtered	136.63	ng/L		-136.63	-100	2.29	ng/L	125.59	ng/L
	Hg0 Unfiltered	26.93	ng/L		-26.93	-100	0.46	ng/L	24.76	ng/L
	HgII Unfiltered	669.61	ng/L		-669.61	-100	10.31	ng/L	615.44	ng/L
	MeHg Unfiltered	2.64	ng/L		-2.64	-100	0.20	ng/L	2.44	ng/L
	HgT Unfiltered	699.18	ng/L		-699.18	-100	10.96	ng/L	642.63	ng/L
	Sediment									
	Hg0 porewater	26.93	ng/L		-26.93	-100	0.46	ng/L	24.757	ng/L
	HgII porewater	73.21	ng/L		-73.21	-100	1.10	ng/L	67.289	ng/L
	MeHg porewater	0.91	ng/L		-0.91	-100	0.04	ng/L	0.842	ng/L
	HgT porewater	101.06	ng/L		-101.06	-100	1.60	ng/L	92.888	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.26	ug/g		-33.26	-100	0.27	ug/g	30.57	ug/g
	MeHg bulk, dry	0.00827	ug/g	0.00422	0.00	-48.97966	0.00	ug/g	0.01	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.499	ug/g	30.58	ug/g
	Trophic Level 3	0.42	ug/g		-0.42	-100	0.064	ug/g	0.39	ug/g
	Trophic Level 4	0.91	ug/g		-0.91	-100	0.140	ug/g	0.85	ug/g
	HI	1.07					0.16		1.00	
	Sensitive Indicator	Mink					Mink		Mink	
	Target C_sed, dry	30.58	ug/g	Note: 8						
	Target C_sed, wet	13.78	ug/g							

Fish

Rate Constants

Process	Media	Value	Units		
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		ratio Sed
1.00E-03	Sediment	1.16E-07	per day		Meth/demeth
Demethylation	Epilimnion	1.16E-08	per day		50.00%
1.00E-03	Hypolimnion	1.16E-07	per day		
2.00E-03	Sediment	2.33E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

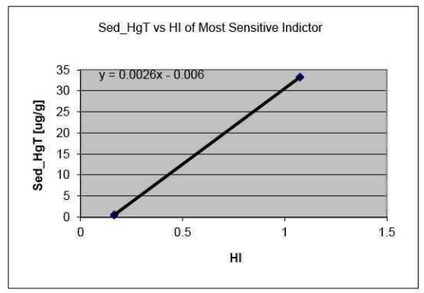
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.51	0.08	0.48
Otter	0.55	0.08	0.51
Mink	**1.07**	0.16	**1.00**
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.98	0.15	0.92
Kingfisher	0.00	0.00	0.00
Wood Duck	0.38	0.06	0.36
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
1.07	33.27
0.16	0.50
m =	36.009
b=	-5.431
Sed_HgT	30.577
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Mink

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.46	0.07	0.427	ng/L

Biota

Trophic Level 1: Phytoplankton	0.09	0.01	0.08	ug Hg/ g wet weight
Trophic Level 2: Insects	0.08	0.01	0.07	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.08	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.42	0.06	0.39	ug Hg/ g wet weight
Trophic Level 4: Bass	0.91	0.14	0.85	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.50	0.08	0.46	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.09	0.01	0.08	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.07	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

	Wildlife Specific Parameters									Contaminated Sediment Calculations								
Animal	**Body Weight** [kg in wet weight]	**Ingestion Rate** [kg wet weight/d]	**Drinking rate** [L/d]	**Percent of Diet from Trophic Level 1 : Phytoplankton and Plants** --	**Percent of Diet from Trophic Level 2 : Insects** --	**Percent of Diet from Trophic Level 2 : Crayfish or Frogs** --	**Percent of Diet from Trophic Level 3 : Fish** --	**Percent of Diet from Trophic Level 4 : Fish** --	**Percent of Diet from nonaquatic sources** --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	39	0	0	0	39	75	0.51
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	31	9	41	75	0.55
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	74	81	75	**1.07**
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	19	7	34	0	59	60	0.98
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	18	5	0	0	0	23	60	0.38
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	9	5000	0.00
Human	**Human Specific Parameters**																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.011	0.00	5.91	0.00	0.00	0.00	6	75	0.08
0.006	0.00	0.00	0.19	4.78	1.39	6	75	0.08
0.007	0.00	0.00	0.60	0.43	11.32	12	75	0.16
0.003	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.033	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.005	0.00	2.84	1.02	5.18	0.00	9	60	0.15
0.008	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.005	2.72	0.80	0.00	0.00	0.00	4	60	0.06
0.000	0.00	0.00	0.07	0.17	1.07	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.068	0.00	35.88	0.00	0.00	0.00	36	75	0.48
0.036	0.00	0.00	1.14	29.02	8.42	39	75	0.51
0.043	0.00	0.00	3.63	2.63	68.74	75	75	**1.00**
0.019	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.201	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.031	0.00	17.25	6.20	31.48	0.00	55	60	0.92
0.048	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.029	16.51	4.86	0.00	0.00	0.00	21	60	0.36
0.000	0.00	0.00	0.43	1.06	6.52	8	5000	0.00
							RfD	
0.008	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.73E-07	0.47
C_HgII_1_Aq			g/m3	9.11E-08	0.09
C_MeHg_1_Aq			g/m3	7.04E-08	0.07
C_Hg0_2_Aq			g/m3	4.60E-07	0.46
C_HgII_2_Aq			g/m3	1.65E-06	1.65
C_MeHg_2_Aq			g/m3	1.79E-07	0.18
C_Hg0_pore			g/m3	4.60E-07	0.46
C_HgII_pore			g/m3	1.10E-06	1.10
C_MeHg_pore			g/m3	4.38E-08	0.04
C_HgT_1_filtered			g/m3	6.34E-07	0.63
C_HgT_2_filtered			g/m3	2.29E-06	2.29
C_HgT_Sed_filtered			g/m3	1.60E-06	1.60
C_Hg0_1_T			g/m3	4.73E-07	0.47
C_HgII_1_T			g/m3	2.69E-06	2.69
C_MeHg_1_T			g/m3	1.36E-07	0.14
C_Hg0_2_T			g/m3	4.60E-07	0.46
C_HgII_2_T			g/m3	1.03E-05	10.31
C_MeHg_2_T			g/m3	1.97E-07	0.20
C_Hg0_sed, bulk			g/m3	3.82E-07	0
C_HgII_1_sed, bulk			g/m3	2.25E-01	224,763
C_MeHg_1_sed, bulk			g/m3	1.79E-04	179
C_Hg0_sed, wet			g/g	2.98E-13	0.000
C_HgII_1_sed, wet			g/g	2.69E-07	0.269
C_MeHg_1_sed, wet			g/g	1.32E-14	0.000
C_HgT_sed,wet			g/g	2.69E-07	0.269
C_Hg0_sed, dry weight			g/g	8.47E-13	0.0000
C_HgII_1_sed, dry weight			g/g	4.99E-07	0.4989
C_MeHg_1_sed, dry weight			g/g	3.96E-10	0.0004
C_HgT_1			g/m3	3.30E-06	3.296
C_HgT_2			g/m3	1.10E-05	10.964
C_HgT_Sed, dry weight			g/g	4.99E-07	0.499

			%Hg0	% HgII	% MeHg
Layer 1	(%Me MeHg_T/Hg_T)		4.14%	81.52%	14.34%
Layer 2			1.79%	94.01%	4.19%
Sediments			0.08%	99.92%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V_1	Volume of Layer 1	Aw*z_1	m3	648,711
V_2	Volume of Layer 2	Aw*z_2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.006
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.087
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.028
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.153
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.028
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.429
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.133
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.757

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{met1} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{met1} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoMe} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{met1} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth,2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{met}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+08	0.00E+00	0.00E+00	-5.25E+03	1.18E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03

b

C Hg0 1 T	-4.89E-01
C HgII 1 T	-6.18E+01
C MeHg 1 T	-1.43E+00
C Hg0 2 T	5.30E+03
C HgII 2 T	5.25E+03
C MeHg 2 T	0.00E+00
C Hg0 sed	0.00E+00
C HgII 1 sed	0.00E+00
C MeHg 1 sed	0.00E+00

Matrix

C Hg0 1 T	4.728E-07
C HgII 1 T	2.687E-06
C MeHg 1 T	1.365E-07
C Hg0 2 T	4.599E-07
C HgII 2 T	1.031E-05
C MeHg 2 T	1.965E-07
C Hg0 sed	3.817E-07
C HgII 1 sed	2.248E-01
C MeHg 1 sed	1.785E-04

Solution

Inverted Matrix

C Hg0 1 T	-8.15E-09	-7.51E-09	-3.03E-09	-7.64E-09	-7.52E-09	-3.06E-09	-7.64E-09	-7.52E-09	-3.06E-09	4.72774E-07
C HgII 1 T	-3.41E-08	-4.29E-08	-1.27E-08	-4.09E-08	-4.25E-08	-1.29E-08	-4.09E-08	-4.25E-08	-1.29E-08	2.68676E-06
C MeHg 1 T	-1.47E-10	-1.83E-10	-8.72E-08	-3.23E-10	-3.65E-10	-8.66E-08	-3.23E-10	-3.75E-10	-8.66E-08	1.36459E-07
C Hg0 2 T	-6.306E-09	-7.327E-09	-2.510E-09	-4.49E-08	-1.32E-08	-2.79E-09	-4.49E-08	-1.32E-08	-2.79E-09	4.59867E-07
C HgII 2 T	-1.324E-07	-1.645E-07	-4.994E-08	-2.90E-07	-3.28E-07	-5.15E-08	-2.90E-07	-3.28E-07	-5.16E-08	1.03079E-05
C MeHg 2 T	-4.770E-10	-5.926E-10	-1.113E-07	-1.04E-09	-1.18E-09	-2.80E-07	-1.04E-09	-1.21E-09	-2.80E-07	1.96543E-07
C Hg0 sed	-5.23E-09	-6.08E-09	-2.08E-09	-3.73E-08	-1.09E-08	-2.31E-09	-3.24E-06	-1.09E-08	-2.31E-09	3.8169E-07
C HgII 1 sed	-2.89E-03	-3.59E-03	-1.09E-03	-6.32E-03	-7.14E-03	-1.12E-03	-6.32E-03	-7.33E-03	-1.13E-03	0.224762892
C MeHg 1 sed	-6.94E-07	-8.62E-07	-8.71E-05	-1.52E-06	-1.72E-06	-2.19E-04	-1.52E-06	-1.76E-06	-4.07E-04	0.000178549

A*x=b

x=b/A

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.006
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.039
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.093
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.744
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.223
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.123
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.037
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.800
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.090
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		4.06E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		2.04E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer.* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer.* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \cdot \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.61
C_HgII_1_Aq			g/m3	2.99E-06	2.99
C_MeHg_1_Aq			g/m3	4.59E-07	0.46
C_Hg0_2_Aq			g/m3	2.69E-05	26.93
C_HgII_2_Aq			g/m3	1.07E-04	107.30
C_MeHg_2_Aq			g/m3	2.40E-06	2.40
C_Hg0_pore			g/m3	2.69E-05	26.93
C_HgII_pore			g/m3	7.32E-05	73.21
C_MeHg_pore			g/m3	9.14E-07	0.91
C_HgT_1_filtered			g/m3	1.91E-05	19.07
C_HgT_2_filtered			g/m3	1.37E-04	136.63
C_HgT_Sed_filtered			g/m3	1.01E-04	101.06
C_Hg0_1_T			g/m3	1.56E-05	15.61
C_HgII_1_T			g/m3	8.83E-05	88.25
C_MeHg_1_T			g/m3	8.90E-07	0.89
C_Hg0_2_T			g/m3	2.69E-05	26.93
C_HgII_2_T			g/m3	6.70E-04	669.61
C_MeHg_2_T			g/m3	2.64E-06	2.64
C_Hg0_sed			g/m3	2.24E-05	22.35
C_HgII_1_sed			g/m3	1.50E+01	14984386.47
C_MeHg_1_sed			g/m3	3.73E-03	3726.18
C_Hg0_sed, wet			g/g	8.44E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.702
C_MeHg_1_sed, wet			g/g	4.46E-09	0.004
C_HgT_sed,wet			g/g	1.17E-05	11.706
C_Hg0_sed, dry weight			g/g	4.96E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.33E-05	33.26
C_MeHg_1_sed, dry weight			g/g	8.27E-09	0.01
C_HgT_1			g/m3	1.05E-04	104.75
C_HgT_2			g/m3	6.99E-04	699.18
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		0.85%	84.25%	14.90%
Layer 2			0.38%	95.77%	3.85%
Sediments			0.02%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.58263%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.65526%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	2.75205%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	2.80992%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	42.93010%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	13.27265%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.04824%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg1}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg1} + Q' \cdot C^w_{MeHg2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{volHg0} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2} + Q' \cdot C^w_{MeHg1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix										x=b/A
	1.561E-05	-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	1.56E-05
	8.825E-05	-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	8.83E-05
	8.905E-07	-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-15	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	8.9E-07
	2.693E-05	-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	2.69E-05
	6.696E-04	-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.00067
	2.635E-06	-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	2.64E-06
	2.235E-05	-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	2.24E-05
	1.498E+01	9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	14.98439
	3.726E-03	-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.003726

A*x=b

C T sed 14.988135 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.97965%
L_T,Hg0	Total Load, Hg0		g/yr	4.89E-01
L_T,HgII	Total Load, HgII		g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg		g/yr	9.36E-01
Rate Constants				
kw_v,Hg0	water column volatilization loss rate constant, Hg0		per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII		per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg		per yr	0.63
kw_oxid_1	water column oxidation rate constant		per yr	564.95
kw_oxid_2	water column oxidation rate constant		per yr	525.60
kw_red_1	water column reduction rate constant, layer 2		per yr	122.63
kw_red_2	water column reduction rate constant, layer 2		per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1		per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2		per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1		per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2		per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1		per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2		per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant		per yr	0.00
kb_oxid	benthic oxidation rate constant		per yr	0.00
kb_red	benthic reduction rate constant		per yr	0.00
kb_methy	benthic methylation rate constant		per yr	0.00
kb_demeth	benthic demethylation rate constant		per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant		per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{sw,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity		m/yr	4792.628412
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	13900.95
TSS_1			mg/L	1.80
TSS+2			mg/L	0.43
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2		L/kg	1.58E+07
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.21E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	2.32E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.44E-05	14.37
C_HgII_1_Aq			g/m3	2.76E-06	2.76
C_MeHg_1_Aq			g/m3	4.27E-07	0.43
C_Hg0_2_Aq			g/m3	2.48E-05	24.76
C_HgII_2_Aq			g/m3	9.86E-05	98.62
C_MeHg_2_Aq			g/m3	2.22E-06	2.22
C_Hg0_pore			g/m3	2.48E-05	24.76
C_HgII_pore			g/m3	6.73E-05	67.29
C_MeHg_pore			g/m3	8.42E-07	0.84
C_HgT_1_filtered			g/m3	1.76E-05	17.55
C_HgT_2_filtered			g/m3	1.26E-04	125.59
C_HgT_Sed_filtered			g/m3	9.29E-05	92.89
C_Hg0_1_T			g/m3	1.44E-05	14.37
C_HgII_1_T			g/m3	8.12E-05	81.22
C_MeHg_1_T			g/m3	8.29E-07	0.83
C_Hg0_2_T			g/m3	2.48E-05	24.76
C_HgII_2_T			g/m3	6.15E-04	615.44
C_MeHg_2_T			g/m3	2.44E-06	2.44
C_Hg0_sed			g/m3	2.05E-05	20.55
C_HgII_1_sed			g/m3	1.38E+01	13,771,621.72
C_MeHg_1_sed			g/m3	3.43E-03	3,434.68
C_Hg0_sed, wet			g/g	7.75E-12	0.00
C_HgII_1_sed, wet			g/g	1.08E-05	10.75
C_MeHg_1_sed, wet			g/g	4.11E-09	0.00
C_HgT_sed,wet			g/g	1.08E-05	10.76
C_Hg0_sed, dry weight			g/g	4.56E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.06E-05	30.57
C_MeHg_1_sed, dry weight			g/g	7.62E-09	0.01
C_HgT_1			g/m3	9.64E-05	96.42
C_HgT_2			g/m3	6.43E-04	642.63
C_HgT_Sed, dry weight			g/g	3.06E-05	30.58
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		0.86%	84.24%	14.90%
Layer 2			0.38%	95.77%	3.85%
Sediments			0.02%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.58263%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.65526%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75205%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			15.26449%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			2.80992%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			42.93010%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			13.27265%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			75.71189%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s,1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,2} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s,2} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{s,2} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	1.437E-05
C_HgII_1_T	3.60E+08	-1.09E+08	9.35E-02	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	8.122E-05
C_MeHg_1_T	0.00E+00	1.61E-01	-1.90E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.42E+00	C_MeHg_1_T	8.285E-07
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	2.476E-05
C_HgII_2_T	0.000E+00	2.250E+07	0.000E+00	2.44E+07	-1.21E+08	3.15E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	6.154E-04
C_MeHg_2_T	0.000E+00	0.000E+00	7.523E+06	0.00E+00	3.15E-01	-1.00E+07	0.00E+00	0.00E+00	5.30E+03	0.00E+00	C_MeHg_2_T	2.435E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	2.055E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.38E+01	C_HgII_1_sed	1.377E+01
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.15E+06	0.00E+00	5.90E-01	-5.31E+03	0.00E+00	C_MeHg_1_sed	3.435E-03

A*x=b

Inverted Matrix

x=b/A

-5.19E-09	-3.83E-09	-1.82E-09	-1.16E-09	-1.95E-10	-1.68E-09	-1.16E-09	1.03E-06	-1.49E-09	1.4E-05
-1.73E-08	-2.21E-08	-5.89E-09	-4.25E-09	-1.10E-09	-5.11E-09	-4.23E-09	5.80E-06	-4.02E-09	8.1E-05
-2.89E-16	-3.88E-16	-8.71E-08	1.16E-15	-2.33E-16	-8.65E-08	1.65E-13	5.11E-08	-8.65E-08	8.3E-07
-1.129E-09	-8.955E-10	-4.014E-10	-3.36E-08	-3.42E-10	-3.78E-10	-3.36E-08	1.79E-06	-4.01E-11	2.5E-05
-3.441E-09	-4.275E-09	2.580E-09	-7.53E-09	-8.51E-09	8.43E-09	-7.39E-09	4.47E-05	1.68E-08	0.00062
-4.582E-16	-6.485E-16	-1.111E-07	3.87E-15	-7.24E-16	-2.80E-07	5.33E-13	1.65E-07	-2.80E-07	2.4E-06
-9.37E-10	-7.43E-10	-3.33E-10	-2.79E-08	-2.84E-10	-3.14E-10	-3.23E-06	1.49E-06	-3.33E-11	2.1E-05
9.37E-10	7.44E-10	8.68E-05	2.79E-08	2.84E-10	2.19E-04	3.23E-06	1.00E+00	4.07E-04	13.7716
-2.54E-13	-4.24E-13	-8.68E-05	6.12E-12	-5.34E-13	-2.19E-04	7.76E-10	2.40E-04	-4.07E-04	0.00343

Target C_sed, wet 13.77507694 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.56114%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01844%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		3.93251%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.29998%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		74.39982%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.34412%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.34651%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		3.70796%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		80.04279%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.97965%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	134.70
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.63
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	122.63
kw_red_2	water column reduction rate constant	per yr	23.27
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for	per yr	0.82
kw_mer	water column *mer* cleavage demethy	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeH	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	1.80
TSS+2		mg/L	0.43
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.58E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.21E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	1.23E+07
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	2.32E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \quad \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{}{C_{dissi}^j + C_{DOC,i}^j} \quad \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = (D_{dry,i} + D_{wet,i}) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left(K_{L,i}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = \left(1.32 + 0.009 \bullet T_a\right)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.58263%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75205%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.65526%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			15.26449%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.80992%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			13.27265%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			42.93010%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			75.71189%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.56114%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			3.93251%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01844%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.04824%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.29998%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			74.39982%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.34412%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.34651%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			80.04279%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			3.70796%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			8.97537%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00041%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.02035%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99959%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.97965%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.17
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.23
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	1,430.88
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1	TSS_1	1.80	mg/L	
Sbio_zoo,1	0.5	TSS_2	0.43	mg/L	
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	1.66E-01				
Sbio_dead,2	2.28E-01				
S_abio, sed	8.42E+04				
S_bio_dead,sed	1.43E+03				
S_sed,total	8.57E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed										
	1	2	3	4	5	6	b		Matrix							x=b/A
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	7.10E+06	S_bio_dead,1	1.66E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.165948
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	2.28E-01	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	0.227765
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	1.43E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	1430.879

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

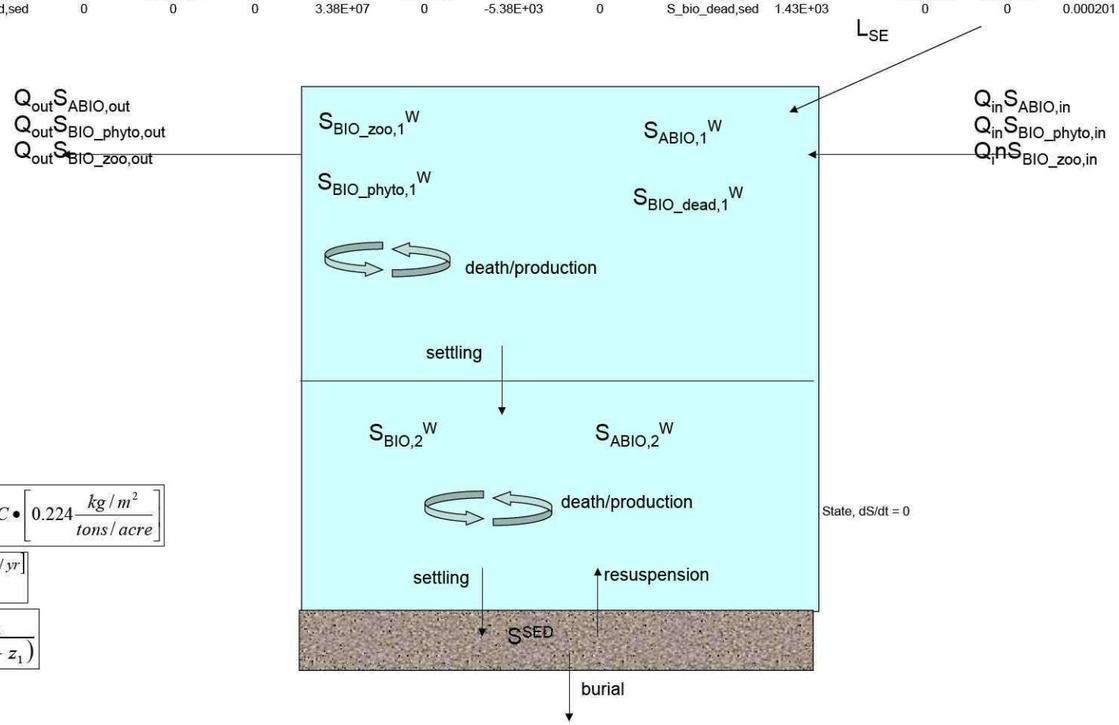
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Mink

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

1 Modeled from Wetzel.

	Oligo	Meso	Eutro	Dystro
Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
Used (mg C/m3)	60	200	500	125
Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

5 Modeled from Wetzel

	50-300	250-1000	>1000	<50-500
Wetzel (mg C/m2/day)				
Used (mg C/m2/day)	175	625	1250	275
Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00583	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.02752		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.02810		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.13273		
k_meth_1	abiotic methylation in layer 1		per yr	2.47E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	6.81E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			5.83E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			2.75E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			2.81E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.33E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	1.44E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	6.81E-06	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weatl		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43* ,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Belted Kingfisher

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	63.07894647
MeHg	7.33E-08	g/m3	0.07332	79.56391716

Total Mercury Concentration in Contaminated Sediment, dry weight	40.7	ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio

HgII	7,182,936	1
MeHg	15,887	1

Kd_bio

HgII	127,696,640	1
MeHg	2,581,565	1

Kd_DOC

HgII	301,427	1
MeHg	310,000	1

	PCT ERROR	CLEANUP
MeHg Filtered	3.02	2.03
HgT Filtered	-32.97	
MeHg Unfilter	96.44	
HgT Unfiltere	185.83	

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	19.35	ng/L		-19.35	-100	0.47	ng/L	1.26	ng/L
	HgII Filtered	2.67	ng/L		-2.67	-100	0.07	ng/L	0.18	ng/L
	MeHg Filtered	0.75	ng/L	0.77	0.02	3.0229168	0.09	ng/L	0.11	ng/L
	HgT Filtered	22.77	ng/L	15.26	-7.51	-32.96994	0.63	ng/L	1.55	ng/L
	Hg0 Unfiltered	19.35	ng/L		-19.35	-100	0.47	ng/L	1.26	ng/L
	HgII Unfiltered	72.38	ng/L		-72.38	-100	1.89	ng/L	4.81	ng/L
	MeHg Unfiltered	1.42	ng/L	2.78	1.36	96.437458	0.16	ng/L	0.22	ng/L
	HgT Unfiltered	93.14	ng/L	266.23	173.09	185.82535	2.53	ng/L	6.29	ng/L
Hypolimnion	Hg0 Filtered	128.71	ng/L		-128.71	-100	1.20	ng/L	6.48	ng/L
	HgII Filtered	231.59	ng/L		-231.59	-100	2.08	ng/L	11.60	ng/L
	MeHg Filtered	4.13	ng/L		-4.13	-100	0.20	ng/L	0.36	ng/L
	HgT Filtered	364.42	ng/L		-364.42	-100	3.47	ng/L	18.44	ng/L
	Hg0 Unfiltered	128.71	ng/L		-128.71	-100	1.20	ng/L	6.48	ng/L
	HgII Unfiltered	710.83	ng/L		-710.83	-100	6.37	ng/L	35.59	ng/L
	MeHg Unfiltered	4.28	ng/L		-4.28	-100	0.21	ng/L	0.38	ng/L
	HgT Unfiltered	843.82	ng/L		-843.82	-100	7.77	ng/L	42.45	ng/L
Sediment										
	Hg0 porewater	128.71	ng/L		-128.71	-100	1.20	ng/L	6.484	ng/L
	HgII porewater	218.67	ng/L		-218.67	-100	1.92	ng/L	10.909	ng/L
	MeHg porewater	2.16	ng/L		-2.16	-100	0.06	ng/L	0.144	ng/L
	HgT porewater	349.54	ng/L		-349.54	-100	3.17	ng/L	17.536	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.69	ug/g		-40.69	-100	0.19	ug/g	2.03	ug/g
	MeHg bulk, dry	0.00795	ug/g	0.00658	0.00	-17.26047	0.00	ug/g	0.00	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.357	ug/g	2.03	ug/g
Fish	Trophic Level 3	0.68	ug/g		-0.68	-100	0.080	ug/g	0.10	ug/g
	Trophic Level 4	1.49	ug/g		-1.49	-100	0.173	ug/g	0.23	ug/g
	HI	6.53					0.76		1.00	
	Sensitive Indicator	Kingfisher					Kingfisher		Kingfisher	
	Target C_sed, dry	2.03	ug/g	Note: 8						
	Target C_sed, wet	0.91	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.16E-07	per day	1.16E-04
	Hypolimnion	1.16E-06	per day	
	Sediment	1.16E-07	per day	
Demethylation	Epilimnion	1.16E-08	per day	
	Hypolimnion	1.16E-07	per day	
	Sediment	2.33E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

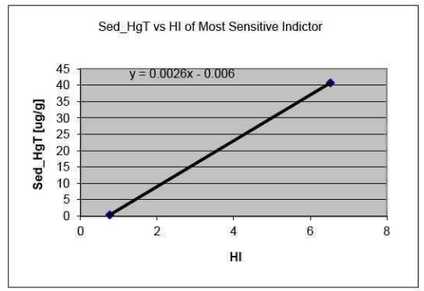
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.84	0.10	0.13
Otter	0.90	0.10	0.14
Mink	**1.75**	0.20	0.27
Great Blue Heron	**3.40**	0.40	0.52
Little Blue Heron	**3.92**	0.46	0.60
Pied-bill Grebe	**1.60**	0.19	0.25
Kingfisher	**6.53**	0.76	**1.00**
Wood Duck	0.62	0.07	0.10
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
6.53	40.70
0.76	0.36
m =	6.996
b=	-4.965
Sed_HgT	2.031
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under tools. Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.75	0.09	0.114	ng/L

Biota

Trophic Level 1: Phytoplankton	0.14	0.02	0.02	ug Hg/ g wet weight
Trophic Level 2: Insects	0.12	0.01	0.02	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.13	0.02	0.02	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.68	0.08	0.10	ug Hg/ g wet weight
Trophic Level 4: Bass	1.49	0.17	0.23	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.81	0.09	0.12	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.14	0.02	0.02	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.13	0.02	0.02	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

Wildlife Specific Parameters

Animal	Body Weight [kg in wet weight]	Ingestion Rate [kg wet weight/d]	Drinking rate [L/d]	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants --	Percent of Diet from Trophic Level 2 : Insects --	Percent of Diet from Trophic Level 2 : Crayfish or Frogs --	Percent of Diet from Trophic Level 3 : Fish --	Percent of Diet from Trophic Level 4 : Fish --	Percent of Diet from nonaquatic sources --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%
Great Blue Heron	2.2	0.509	0.1	0%	5%	10%	50%	35%	0%
Little Blue Heron	0.34	0.147	0.16	0%	25%	0%	75%	0%	0%
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%
Kingfisher	0.15	0.086	0.017	0%	0%	0%	100%	0%	0%
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%

Contaminated Sediment Calculations

Animal	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0	0	63	0	0	0	63	75	0.84
Otter	0	0	0	2	51	15	67	75	0.90
Mink	0	0	0	6	5	120	131	75	**1.75**
Great Blue Heron	0	0	1	3	79	120	204	60	**3.40**
Little Blue Heron	0	0	13	0	222	0	235	60	**3.92**
Pied-bill Grebe	0	0	30	11	55	0	96	60	**1.60**
Kingfisher	0	0	0	0	392	0	392	60	**6.53**
Wood Duck	0	29	9	0	0	0	37	60	0.62
Alligator	0	0	0	1	2	11	14	5000	0.00

Human

Human Specific Parameters

																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution 5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.014	0.00	7.31	0.00	0.00	0.00	7	75	0.10
0.007	0.00	0.00	0.23	5.91	1.72	8	75	0.10
0.009	0.00	0.00	0.74	0.54	14.01	15	75	0.20
0.004	0.00	0.17	0.36	9.21	14.04	24	60	0.40
0.041	0.00	1.57	0.00	25.82	0.00	27	60	0.46
0.006	0.00	3.52	1.26	6.42	0.00	11	60	0.19
0.010	0.00	0.00	0.00	45.65	0.00	46	60	0.76
0.006	3.36	0.99	0.00	0.00	0.00	4	60	0.07
0.000	0.00	0.00	0.09	0.22	1.33	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.018	0.00	9.61	0.00	0.00	0.00	10	75	0.13
0.010	0.00	0.00	0.31	7.77	2.26	10	75	0.14
0.011	0.00	0.00	0.97	0.70	18.42	20	75	0.27
0.005	0.00	0.22	0.48	12.11	18.45	31	60	0.52
0.054	0.00	2.07	0.00	33.93	0.00	36	60	0.60
0.008	0.00	4.62	1.66	8.43	0.00	15	60	0.25
0.013	0.00	0.00	0.00	60.00	0.00	60	60	**1.00**
0.008	4.42	1.30	0.00	0.00	0.00	6	60	0.10
0.000	0.00	0.00	0.12	0.28	1.75	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Belted Kingfisher

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)
HgII	mean	3.8	5.3	4.9	5.4
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6
	n	17	35	2	3
MeHg	mean	2.8	4.9	3.9	5
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5
	n	11	2		

Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
			199526.23				
630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	1584893.2	100000	316227.77	8	635462.6		12,679,146
			630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.38

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.75E-07	0.47
C_HgII_1_Aq			g/m3	6.96E-08	0.07
C_MeHg_1_Aq			g/m3	8.71E-08	0.09
C_Hg0_2_Aq			g/m3	1.20E-06	1.20
C_HgII_2_Aq			g/m3	2.08E-06	2.08
C_MeHg_2_Aq			g/m3	2.00E-07	0.20
C_Hg0_pore			g/m3	1.20E-06	1.20
C_HgII_pore			g/m3	1.92E-06	1.92
C_MeHg_pore			g/m3	5.66E-08	0.06
C_HgT_1_filtered			g/m3	6.31E-07	0.63
C_HgT_2_filtered			g/m3	3.47E-06	3.47
C_HgT_Sed_filtered			g/m3	3.17E-06	3.17
C_Hg0_1_T			g/m3	4.75E-07	0.47
C_HgII_1_T			g/m3	1.89E-06	1.89
C_MeHg_1_T			g/m3	1.65E-07	0.16
C_Hg0_2_T			g/m3	1.20E-06	1.20
C_HgII_2_T			g/m3	6.37E-06	6.37
C_MeHg_2_T			g/m3	2.07E-07	0.21
C_Hg0_sed, bulk			g/m3	9.92E-07	1
C_HgII_1_sed, bulk			g/m3	1.61E-01	160,828
C_MeHg_1_sed, bulk			g/m3	9.38E-05	94
C_Hg0_sed, wet			g/g	7.75E-13	0.000
C_HgII_1_sed, wet			g/g	1.93E-07	0.193
C_MeHg_1_sed, wet			g/g	8.52E-15	0.000
C_HgT_sed,wet			g/g	1.93E-07	0.193
C_Hg0_sed, dry weight			g/g	2.20E-12	0.0000
C_HgII_1_sed, dry weight			g/g	3.57E-07	0.3570
C_MeHg_1_sed, dry weight			g/g	2.08E-10	0.0002
C_HgT_1			g/m3	2.53E-06	2.530
C_HgT_2			g/m3	7.77E-06	7.773
C_HgT_Sed, dry weight			g/g	3.57E-07	0.357
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		6.52%	74.72%	18.76%
Layer 2			2.66%	81.96%	15.37%
Sediments			0.06%	99.94%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{vol,Hg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abio,Hg0} \cdot A_w - v_{s,B} \cdot f^{w,1}_{bio,Hg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{vol,HgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{met,1} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abio,HgII} \cdot A_w - v_{s,B} \cdot f^{w,1}_{bio,HgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg1}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{met,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{vol,MeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abio,MeHg} \cdot A_w - v_{s,B} \cdot f^{w,1}_{bio,MeHg} \cdot A_w\right] \cdot C^w_{MeHg1} + Q' \cdot C^w_{MeHg2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abio,Hg0} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bio,Hg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,Hg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aq,Hg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sed,Hg0} \cdot A_w\right] \cdot C^{sed}_{aq,Hg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red,2} \cdot V_w - kw_{met,2} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abio,HgII} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bio,HgII} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,HgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aq,HgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sed,HgII} \cdot A_w\right] \cdot C^{sed}_{aq,HgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth,2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aq,Hg0} + \left(v_{s,A} \cdot f^{w,2}_{abio,Hg0} + v_{s,B} \cdot f^{w,2}_{bio,Hg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aq,Hg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,Hg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aq,HgII} + \left(v_{s,A} \cdot f^{w,2}_{abio,HgII} + v_{s,B} \cdot f^{w,2}_{bio,HgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aq,HgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,HgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aq,MeHg} + \left(v_{s,A} \cdot f^{w,2}_{abio,MeHg} + v_{s,B} \cdot f^{w,2}_{bio,MeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aq,MeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,MeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	1.12E+08	-6.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.08E+08	0.00E+00	0.00E+00	-4.29E+03	9.64E-01
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	4.82E-01	-4.40E+03

Matrix b

C Hg0 1 T	4.746E-07
C HgII 1 T	1.890E-06
C MeHg 1 T	1.649E-07
C Hg0 2 T	1.195E-06
C HgII 2 T	6.371E-06
C MeHg 2 T	2.071E-07
C Hg0 sed	9.919E-07
C HgII 1 sed	1.608E-01
C MeHg 1 sed	9.382E-05

Solution Inverted Matrix x=b/A

Matrix

C Hg0 1 T	-1.21E-08	-1.13E-08	-4.94E-09	-1.15E-08	-1.14E-08	-5.43E-09	-1.15E-08	-1.14E-08	-5.43E-09	4.74599E-07
C HgII 1 T	-2.73E-08	-4.52E-08	-1.18E-08	-4.04E-08	-4.24E-08	-1.39E-08	-4.04E-08	-4.24E-08	-1.39E-08	1.89003E-06
C MeHg 1 T	-1.66E-10	-2.64E-10	-1.54E-07	-6.61E-10	-7.36E-10	-1.43E-07	-6.61E-10	-7.52E-10	-1.43E-07	1.64944E-07
C Hg0 2 T	-1.859E-08	-2.847E-08	-1.157E-08	-1.13E-07	-7.67E-08	-1.91E-08	-1.13E-07	-7.67E-08	-1.91E-08	1.19505E-06
C HgII 2 T	-9.578E-08	-1.520E-07	-5.127E-08	-3.81E-07	-4.24E-07	-7.59E-08	-3.81E-07	-4.24E-07	-7.60E-08	6.37108E-06
C MeHg 2 T	-5.423E-10	-8.609E-10	-1.718E-07	-2.16E-09	-2.40E-09	-4.66E-07	-2.16E-09	-2.45E-09	-4.66E-07	2.07147E-07
C Hg0 sed	-1.54E-08	-2.36E-08	-9.60E-09	-9.36E-08	-6.37E-08	-1.59E-08	-4.01E-06	-6.37E-08	-1.59E-08	9.91889E-07
C HgII 1 sed	-2.42E-03	-3.84E-03	-1.29E-03	-9.61E-03	-1.07E-02	-1.92E-03	-9.61E-03	-1.09E-02	-1.92E-03	0.16082824
C MeHg 1 sed	-4.64E-07	-7.37E-07	-6.33E-05	-1.84E-06	-2.05E-06	-1.72E-04	-1.84E-06	-2.10E-06	-3.99E-04	9.38187E-05

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.004
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.050
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.101
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.229
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.808
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.229
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.050
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.014
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.624
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.036
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		9.90E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		5.01E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		9.99E-01
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	11351.43
TSS_1		mg/L	1.65
TSS+2		mg/L	0.21
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org-org,i}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}}}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.94E-05	19.35
C_HgII_1_Aq			g/m3	2.67E-06	2.67
C_MeHg_1_Aq			g/m3	7.47E-07	0.75
C_Hg0_2_Aq			g/m3	1.29E-04	128.71
C_HgII_2_Aq			g/m3	2.32E-04	231.59
C_MeHg_2_Aq			g/m3	4.13E-06	4.13
C_Hg0_pore			g/m3	1.29E-04	128.71
C_HgII_pore			g/m3	2.19E-04	218.67
C_MeHg_pore			g/m3	2.16E-06	2.16
C_HgT_1_filtered			g/m3	2.28E-05	22.77
C_HgT_2_filtered			g/m3	3.64E-04	364.42
C_HgT_Sed_filtered			g/m3	3.50E-04	349.54
C_Hg0_1_T			g/m3	1.94E-05	19.35
C_HgII_1_T			g/m3	7.24E-05	72.38
C_MeHg_1_T			g/m3	1.42E-06	1.42
C_Hg0_2_T			g/m3	1.29E-04	128.71
C_HgII_2_T			g/m3	7.11E-04	710.83
C_MeHg_2_T			g/m3	4.28E-06	4.28
C_Hg0_sed			g/m3	1.07E-04	106.83
C_HgII_1_sed			g/m3	1.83E+01	18331660.50
C_MeHg_1_sed			g/m3	3.58E-03	3582.68
C_Hg0_sed, wet			g/q	4.03E-11	0.000
C_HgII_1_sed, wet			g/q	1.43E-05	14.316
C_MeHg_1_sed, wet			g/q	4.29E-09	0.004
C_HgT_sed,wet			g/q	1.43E-05	14.320
C_Hg0_sed, dry weight			g/q	2.37E-10	0.00
C_HgII_1_sed, dry weight			g/q	4.07E-05	40.69
C_MeHg_1_sed, dry weight			g/q	7.95E-09	0.01
C_HgT_1			g/m3	9.31E-05	93.14
C_HgT_2			g/m3	8.44E-04	843.82
C_HgT_Sed			g/g	4.07E-05	40.70
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		1.52%	77.70%	20.78%
Layer 2			0.51%	84.24%	15.25%
Sediments			0.02%	99.98%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.63276%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.86115%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	5.59528%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.05171%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	43.95131%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	26.98508%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03204%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photordd} V_w\right] \cdot C^w_{MeHg,1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg,1} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photordd} V_w - v_{s,1} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg,1} + Q' \cdot C^w_{MeHg,2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} V_w + kw_{photordd} V_w\right] \cdot C^w_{MeHg,2} + \left[-Q' - kw_{oxid} V_w - v_{s,1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot A_w \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg,2} + \left[-Q' - kw_{red,2} \cdot V_w - kw_{meth} \cdot V_w - v_{s,1} \cdot f^{w,2}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHgII} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII}\right] \cdot A_w \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg,2}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photordd} \cdot V_w - v_{s,1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg,2} + Q' \cdot C^w_{MeHg,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T
C_HgII_1_T	1.12E+08	-6.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E-01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	4.82E-01	-4.40E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix									x=b/A	
1.935E-05	-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	1.94E-05	C_Hg0_1_T
7.238E-05	-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	7.24E-05	C_HgII_1_T
1.415E-06	-1.97E-16	-3.86E-16	-1.54E-07	1.96E-15	-5.89E-16	-1.43E-07	2.72E-13	6.88E-08	-1.43E-07	1.42E-06	C_MeHg_1_T
1.287E-04	-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	0.000129	C_Hg0_2_T
7.108E-04	-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.000711	C_HgII_2_T
4.283E-06	-3.476E-16	-7.619E-16	-1.715E-07	6.42E-15	-1.91E-15	-4.65E-07	8.86E-13	2.24E-07	-4.65E-07	4.28E-06	C_MeHg_2_T
1.068E-04	-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	0.000107	C_Hg0_sed
1.833E+01	1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	18.33166	C_HgII_1_sed
3.583E-03	1.97E-14	-1.41E-13	-6.31E-05	6.48E-12	-5.53E-13	-1.71E-04	7.59E-10	1.92E-04	-3.98E-04	0.003583	C_MeHg_1_sed

C_T_sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1 - \theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \times 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	1.65
TSS+2			mg/L	0.21
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2		L/kg	1.59E+07
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.43E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	1.80E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{physto}^{j}C_{physto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{physto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.26E-06	1.26
C_HgII_1_Aq			g/m3	1.77E-07	0.18
C_MeHg_1_Aq			g/m3	1.14E-07	0.11
C_Hg0_2_Aq			g/m3	6.48E-06	6.48
C_HgII_2_Aq			g/m3	1.16E-05	11.60
C_MeHg_2_Aq			g/m3	3.62E-07	0.36
C_Hg0_pore			g/m3	6.48E-06	6.48
C_HgII_pore			g/m3	1.09E-05	10.91
C_MeHg_pore			g/m3	1.44E-07	0.14
C_HgT_1_filtered			g/m3	1.55E-06	1.55
C_HgT_2_filtered			g/m3	1.84E-05	18.44
C_HgT_Sed_filtered			g/m3	1.75E-05	17.54
C_Hg0_1_T			g/m3	1.26E-06	1.26
C_HgII_1_T			g/m3	4.81E-06	4.81
C_MeHg_1_T			g/m3	2.17E-07	0.22
C_Hg0_2_T			g/m3	6.48E-06	6.48
C_HgII_2_T			g/m3	3.56E-05	35.59
C_MeHg_2_T			g/m3	3.76E-07	0.38
C_Hg0_sed			g/m3	5.38E-06	5.38
C_HgII_1_sed			g/m3	9.15E-01	914,501.16
C_MeHg_1_sed			g/m3	2.39E-04	238.53
C_Hg0_sed, wet			g/g	2.03E-12	0.00
C_HgII_1_sed, wet			g/g	7.14E-07	0.71
C_MeHg_1_sed, wet			g/g	2.86E-10	0.00
C_HgT_sed,wet			g/g	7.14E-07	0.71
C_Hg0_sed, dry weight			g/g	1.19E-11	0.00
C_HgII_1_sed, dry weight			g/g	2.03E-06	2.03
C_MeHg_1_sed, dry weight			g/g	5.29E-10	0.00
C_HgT_1			g/m3	6.29E-06	6.29
C_HgT_2			g/m3	4.25E-05	42.45
C_HgT_Sed, dry weight			g/g	2.03E-06	2.03
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.45%	76.55%	20.00%
Layer 2			0.89%	83.84%	15.27%
Sediments			0.03%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			3.05171%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			26.98508%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{s,B} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHgII} A_w - v_{s,B} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s,A} \cdot f^{w,1}_{abioMeHg} A_w - v_{s,B} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioHgII} A_w - v_{s,B} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioMeHg} A_w - v_{s,B} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,A} \cdot f^{w,2}_{abioHg0} + v_{s,B} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,A} \cdot f^{w,2}_{abioHgII} + v_{s,B} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,A} \cdot f^{w,2}_{abioMeHg} + v_{s,B} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	1.258E-06
C_HgII_1_T	1.12E+08	-8.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	4.814E-06
C_MeHg_1_T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	2.168E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	6.484E-06
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	3.559E-05
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00	C_MeHg_2_T	3.762E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	5.382E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	9.15E-01	C_HgII_1_sed	9.145E-01
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	4.82E-01	-4.40E+03	0.00E+00	C_MeHg_1_sed	2.385E-04

Inverted Matrix

-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	1.3E-06
-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	4.8E-06
-1.97E-16	-3.86E-16	-1.54E-07	1.96E-15	-5.89E-16	-1.43E-07	2.72E-13	6.88E-08	-1.43E-07	2.2E-07
-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	6.5E-06
-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	3.6E-05
-3.476E-16	-7.619E-16	-1.715E-07	6.42E-15	-1.91E-15	-4.65E-07	8.86E-13	2.24E-07	-4.65E-07	3.8E-07
-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	5.4E-06
1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	0.9145
1.97E-14	-1.41E-13	-6.31E-05	6.48E-12	-5.53E-13	-1.71E-04	7.59E-10	1.92E-04	-3.98E-04	0.00024

x=b/A

A*x=b

Target C_sed, wet 0.914745069 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	388.36
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	246.95
kw_red_2	water column reduction rate constant	per yr	107.40
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for	per yr	6.43
kw_mer	water column *mer* cleavage demethy	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeH(	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	1.65
TSS+2		mg/L	0.21
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{}{C_{diss,i}^j + C_{DOC,i}^j} \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = (D_{dry,i} + D_{wet,i}) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05171%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			26.98508%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.38210%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.01537%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01183%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			10.10022%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			80.80179%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			5.03141%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			62.40427%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			1.42443%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.94994%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.06
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.09
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	548.69
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1		TSS_1	1.65	mg/L
Sbio_zoo,1	0.5		TSS_2	0.21	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	6.23E-02				
Sbio_dead,2	8.73E-02				
S_abio, sed	5.28E+04				
S_bio_dead,sed	5.49E+02				
S_sed,total	5.34E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			Solution	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b		Matrix							
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	2.01E+06	S_bio_dead,1	6.23E-02	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.062268
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	8.73E-02	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.08734
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	5.49E+02	0	0	0.000273	-2.50E-04	0	-3.07E-04	548.6925

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

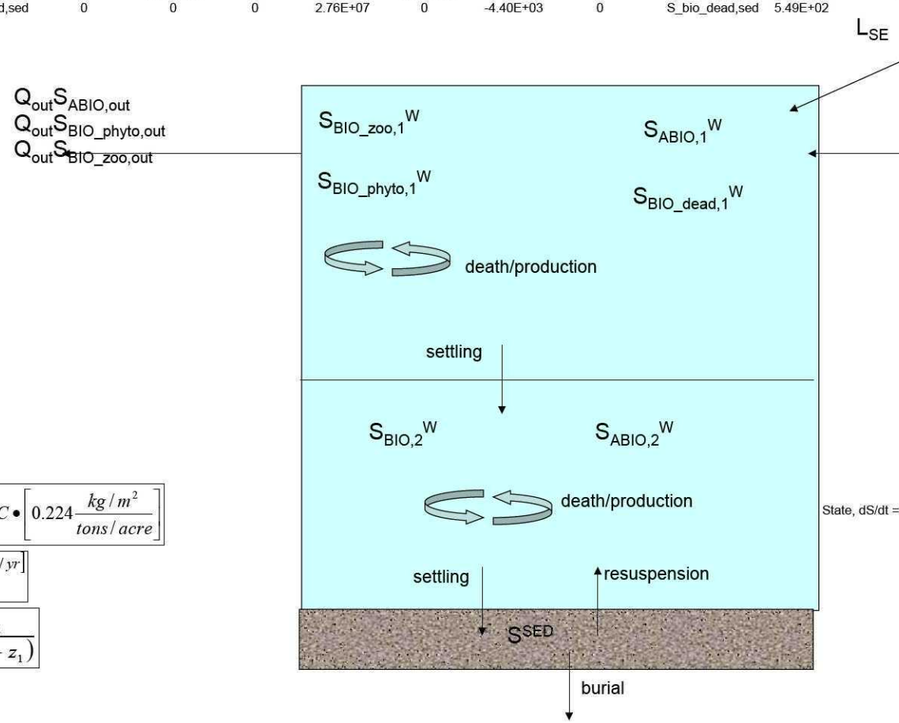
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00633	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.05595		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03052		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.26985		
k_meth_1	abiotic methylation in layer 1		per yr	2.69E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.38E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			6.33E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.60E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			2.70E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	1.56E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.38E-05	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability.
Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weatl		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 UV-B is modeled as being 0.5% of visible light.
check?

1 $$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{.86}$$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Belted Kingfisher

Varied Diet

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	63.07894647
MeHg	7.33E-08	g/m3	0.07332	79.56391716

Total Mercury Concentration in Contaminated Sediment, dry weight	40.7	ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio

HgII	7,182,936	1
MeHg	15,887	1

Kd_bio

HgII	127,696,640	1
MeHg	2,581,565	1

Kd_DOC

HgII	301,427	1
MeHg	310,000	1

	PCT ERROR	CLEANUP
MeHg Filtered	3.02	9.69
HgT Filtered	-32.97	
MeHg Unfilter	96.44	
HgT Unfiltere	185.83	

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	19.35	ng/L		-19.35	-100	0.47	ng/L	4.84	ng/L
	HgII Filtered	2.67	ng/L		-2.67	-100	0.07	ng/L	0.67	ng/L
	MeHg Filtered	0.75	ng/L	0.77	0.02	3.0229168	0.09	ng/L	0.24	ng/L
	HgT Filtered	22.77	ng/L	15.26	-7.51	-32.96994	0.63	ng/L	5.75	ng/L
	Hg0 Unfiltered	19.35	ng/L		-19.35	-100	0.47	ng/L	4.84	ng/L
	HgII Unfiltered	72.38	ng/L		-72.38	-100	1.89	ng/L	18.21	ng/L
	MeHg Unfiltered	1.42	ng/L	2.78	1.36	96.437458	0.16	ng/L	0.45	ng/L
	HgT Unfiltered	93.14	ng/L	266.23	173.09	185.82535	2.53	ng/L	23.50	ng/L
Hypolimnion	Hg0 Filtered	128.71	ng/L		-128.71	-100	1.20	ng/L	30.71	ng/L
	HgII Filtered	231.59	ng/L		-231.59	-100	2.08	ng/L	55.20	ng/L
	MeHg Filtered	4.13	ng/L		-4.13	-100	0.20	ng/L	1.11	ng/L
	HgT Filtered	364.42	ng/L		-364.42	-100	3.47	ng/L	87.02	ng/L
	Hg0 Unfiltered	128.71	ng/L		-128.71	-100	1.20	ng/L	30.71	ng/L
	HgII Unfiltered	710.83	ng/L		-710.83	-100	6.37	ng/L	169.43	ng/L
	MeHg Unfiltered	4.28	ng/L		-4.28	-100	0.21	ng/L	1.15	ng/L
	HgT Unfiltered	843.82	ng/L		-843.82	-100	7.77	ng/L	201.28	ng/L
Sediment										
	Hg0 porewater	128.71	ng/L		-128.71	-100	1.20	ng/L	30.709	ng/L
	HgII porewater	218.67	ng/L		-218.67	-100	1.92	ng/L	52.087	ng/L
	MeHg porewater	2.16	ng/L		-2.16	-100	0.06	ng/L	0.544	ng/L
	HgT porewater	349.54	ng/L		-349.54	-100	3.17	ng/L	83.340	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.69	ug/g		-40.69	-100	0.19	ug/g	9.69	ug/g
	MeHg bulk, dry	0.00795	ug/g	0.00658	0.00	-17.26047	0.00	ug/g	0.00	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.357	ug/g	9.69	ug/g
Fish	Trophic Level 3	0.68	ug/g		-0.68	-100	0.080	ug/g	0.22	ug/g
	Trophic Level 4	1.49	ug/g		-1.49	-100	0.173	ug/g	0.48	ug/g
	HI	3.11					0.36		1.00	
	Sensitive Indicator	Kingfisher					Kingfisher		Kingfisher	
	Target C_sed, dry	9.69	ug/g	Note: 8						
	Target C_sed, wet	4.37	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.16E-07	per day	1.16E-04
	Hypolimnion	1.16E-06	per day	
	Sediment	1.16E-07	per day	
Demethylation	Epilimnion	1.16E-08	per day	
	Hypolimnion	1.16E-07	per day	
	Sediment	2.33E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

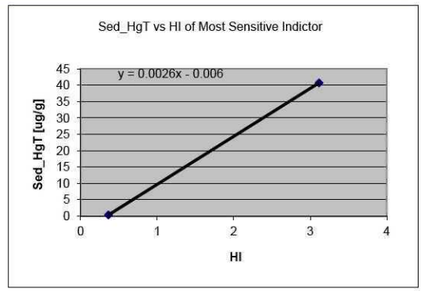
Human and Wildlife Exposure Risk Results

8,594

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.84	0.10	0.27
Otter	0.90	0.10	0.29
Mink	**1.75**	0.20	0.56
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	**1.60**	0.19	0.51
Kingfisher	**3.11**	0.36	**1.00**
Wood Duck	0.62	0.07	0.20
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
3.11	40.70
0.36	0.36
m =	14.660
b=	-4.965
Sed_HgT	9.695
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under tools. Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.75	0.09	0.240	ng/L

Biota

Trophic Level 1: Phytoplankton	0.14	0.02	0.05	ug Hg/ g wet weight
Trophic Level 2: Insects	0.12	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.13	0.02	0.04	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.68	0.08	0.22	ug Hg/ g wet weight
Trophic Level 4: Bass	1.49	0.17	0.48	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.81	0.09	0.26	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.14	0.02	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.13	0.02	0.04	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Body Weight	Ingestion Rate	Drinking rate	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants	Percent of Diet from Trophic Level 2 : Insects	Percent of Diet from Trophic Level 2 : Crayfish or Frogs	Percent of Diet from Trophic Level 3 : Fish	Percent of Diet from Trophic Level 4 : Fish	Percent of Diet from nonaquatic sources	Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Insects	Potential Dose from Trophic Level 2: Crayfish	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
Animal	[kg in wet weight]	[kg wet weight/d]	[L/d]	--	--	--	--	--	--	[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	63	0	0	0	63	75	0.84
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	2	51	15	67	75	0.90
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	6	5	120	131	75	**1.75**
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	30	11	55	0	96	60	**1.60**
Kingfisher	0.15	0.086	0.017	0%	0%	18%	23%	10%	50%	0	0	0	13	88	85	187	60	**3.11**
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	29	9	0	0	0	37	60	0.62
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	1	2	11	14	5000	0.00
Human																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.014	0.00	7.31	0.00	0.00	0.00	7	75	0.10
0.007	0.00	0.00	0.23	5.91	1.72	8	75	0.10
0.009	0.00	0.00	0.74	0.54	14.01	15	75	0.20
0.004	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.041	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.006	0.00	3.52	1.26	6.42	0.00	11	60	0.19
0.010	0.00	0.00	1.57	10.27	9.94	22	60	0.36
0.006	3.36	0.99	0.00	0.00	0.00	4	60	0.07
0.000	0.00	0.00	0.09	0.22	1.33	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.038	0.00	20.14	0.00	0.00	0.00	20	75	0.27
0.020	0.00	0.00	0.64	16.29	4.73	22	75	0.29
0.024	0.00	0.00	2.04	1.48	38.59	42	75	0.56
0.011	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.113	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.017	0.00	9.69	3.48	17.67	0.00	31	60	0.51
0.027	0.00	0.00	4.33	28.29	27.38	60	60	**1.00**
0.016	9.27	2.73	0.00	0.00	0.00	12	60	0.20
0.000	0.00	0.00	0.24	0.60	3.66	4	5000	0.00
							RfD	
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Belted Kingfisher – Varied Diet

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893.2	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.75E-07	0.47
C_HgII_1_Aq			g/m3	6.96E-08	0.07
C_MeHg_1_Aq			g/m3	8.71E-08	0.09
C_Hg0_2_Aq			g/m3	1.20E-06	1.20
C_HgII_2_Aq			g/m3	2.08E-06	2.08
C_MeHg_2_Aq			g/m3	2.00E-07	0.20
C_Hg0_pore			g/m3	1.20E-06	1.20
C_HgII_pore			g/m3	1.92E-06	1.92
C_MeHg_pore			g/m3	5.66E-08	0.06
C_HgT_1_filtered			g/m3	6.31E-07	0.63
C_HgT_2_filtered			g/m3	3.47E-06	3.47
C_HgT_Sed_filtered			g/m3	3.17E-06	3.17
C_Hg0_1_T			g/m3	4.75E-07	0.47
C_HgII_1_T			g/m3	1.89E-06	1.89
C_MeHg_1_T			g/m3	1.65E-07	0.16
C_Hg0_2_T			g/m3	1.20E-06	1.20
C_HgII_2_T			g/m3	6.37E-06	6.37
C_MeHg_2_T			g/m3	2.07E-07	0.21
C_Hg0_sed, bulk			g/m3	9.92E-07	1
C_HgII_1_sed, bulk			g/m3	1.61E-01	160,828
C_MeHg_1_sed, bulk			g/m3	9.38E-05	94
C_Hg0_sed, wet			g/g	7.75E-13	0.000
C_HgII_1_sed, wet			g/g	1.93E-07	0.193
C_MeHg_1_sed, wet			g/g	8.52E-15	0.000
C_HgT_sed,wet			g/g	1.93E-07	0.193
C_Hg0_sed, dry weight			g/g	2.20E-12	0.0000
C_HgII_1_sed, dry weight			g/g	3.57E-07	0.3570
C_MeHg_1_sed, dry weight			g/g	2.08E-10	0.0002
C_HgT_1			g/m3	2.53E-06	2.530
C_HgT_2			g/m3	7.77E-06	7.773
C_HgT_Sed, dry weight			g/g	3.57E-07	0.357
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		6.52%	74.72%	18.76%
Layer 2			2.66%	81.96%	15.37%
Sediments			0.06%	99.94%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth,2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9
C Hg0 1 T	**-1.90E+08**	**4.54E+07**	**2.39E+06**	**3.02E+06**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	**1.12E+08**	**-6.02E+07**	**2.88E-02**	0.00E+00	**3.02E+06**	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	**4.94E-02**	**-9.84E+06**	0.00E+00	0.00E+00	**3.02E+06**	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	**3.018E+06**	0.000E+00	0.000E+00	**-2.31E+07**	**4.06E+06**	**2.43E+05**	**2.55E+05**	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	**1.134E+07**	0.000E+00	**1.99E+07**	**-1.15E+08**	**5.24E-01**	0.00E+00	**4.29E+03**	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	**3.626E+06**	0.00E+00	**5.24E-01**	**-4.88E+06**	0.00E+00	0.00E+00	**4.40E+03**
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	**2.12E+05**	0.00E+00	0.00E+00	**-2.55E+05**	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	**1.08E+08**	0.00E+00	0.00E+00	**-4.29E+03**	**9.64E-01**
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	**1.62E+06**	0.00E+00	**4.82E-01**	**-4.40E+03**

b

C Hg0 1 T	**-3.99E-01**
C HgII 1 T	**-4.13E+01**
C MeHg 1 T	**-9.97E-01**
C Hg0 2 T	0.00E+00
C HgII 2 T	0.00E+00
C MeHg 2 T	0.00E+00
C Hg0 sed	0.00E+00
C HgII 1 sed	0.00E+00
C MeHg 1 sed	0.00E+00

Matrix

C Hg0 1 T	4.746E-07
C HgII 1 T	1.890E-06
C MeHg 1 T	1.649E-07
C Hg0 2 T	1.195E-06
C HgII 2 T	6.371E-06
C MeHg 2 T	2.071E-07
C Hg0 sed	9.919E-07
C HgII 1 sed	1.608E-01
C MeHg 1 sed	9.382E-05

Solution Inverted Matrix x=b/A

C Hg0 1 T	**-1.21E-08**	**-1.13E-08**	**-4.94E-09**	**-1.15E-08**	**-1.14E-08**	**-5.43E-09**	**-1.15E-08**	**-1.14E-08**	**-5.43E-09**	4.74599E-07
C HgII 1 T	**-2.73E-08**	**-4.52E-08**	**-1.18E-08**	**-4.04E-08**	**-4.24E-08**	**-1.39E-08**	**-4.04E-08**	**-4.24E-08**	**-1.39E-08**	1.89003E-06
C MeHg 1 T	**-1.66E-10**	**-2.64E-10**	**-1.54E-07**	**-6.61E-10**	**-7.36E-10**	**-1.43E-07**	**-6.61E-10**	**-7.52E-10**	**-1.43E-07**	1.64944E-07
C Hg0 2 T	**-1.859E-08**	**-2.847E-08**	**-1.157E-08**	**-1.13E-07**	**-7.67E-08**	**-1.91E-08**	**-1.13E-07**	**-7.67E-08**	**-1.91E-08**	1.19505E-06
C HgII 2 T	**-9.578E-08**	**-1.520E-07**	**-5.127E-08**	**-3.81E-07**	**-4.24E-07**	**-7.59E-08**	**-3.81E-07**	**-4.24E-07**	**-7.60E-08**	6.37108E-06
C MeHg 2 T	**-5.423E-10**	**-8.609E-10**	**-1.718E-07**	**-2.16E-09**	**-2.40E-09**	**-4.66E-07**	**-2.16E-09**	**-2.45E-09**	**-4.66E-07**	2.07147E-07
C Hg0 sed	**-1.54E-08**	**-2.36E-08**	**-9.60E-09**	**-9.36E-08**	**-6.37E-08**	**-1.59E-08**	**-4.01E-06**	**-6.37E-08**	**-1.59E-08**	9.91889E-07
C HgII 1 sed	**-2.42E-03**	**-3.84E-03**	**-1.29E-03**	**-9.61E-03**	**-1.07E-02**	**-1.92E-03**	**-9.61E-03**	**-1.09E-02**	**-1.92E-03**	0.16082824
C MeHg 1 sed	**-4.64E-07**	**-7.37E-07**	**-6.33E-05**	**-1.84E-06**	**-2.05E-06**	**-1.72E-04**	**-1.84E-06**	**-2.10E-06**	**-3.99E-04**	9.38187E-05

A*x=b

Symbol	Parameter	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.006
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.089
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.056
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.162
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.031
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.440
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.270
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.802

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.004
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.050
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.101
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.229
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.808
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.229
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.050
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.014
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.624
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.036
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		9.90E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		5.01E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		9.99E-01
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer*. cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer*. cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	11351.43
TSS_1		mg/L	1.65
TSS+2		mg/L	0.21
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \Big/ \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS} = \frac{C_{filtered,i}^{j}}{C_{diss,i}^{j}+C_{DOC,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C Hg0 1 Aq			g/m3	1.94E-05	19.35
C HgII 1 Aq			g/m3	2.67E-06	2.67
C MeHg 1 Aq			g/m3	7.47E-07	0.75
C Hg0 2 Aq			g/m3	1.29E-04	128.71
C HgII 2 Aq			g/m3	2.32E-04	231.59
C MeHg 2 Aq			g/m3	4.13E-06	4.13
C Hg0 pore			g/m3	1.29E-04	128.71
C HgII pore			g/m3	2.19E-04	218.67
C MeHg pore			g/m3	2.16E-06	2.16
C HgT 1 filtered			g/m3	2.28E-05	22.77
C HgT 2 filtered			g/m3	3.64E-04	364.42
C HgT Sed filtered			g/m3	3.50E-04	349.54
C Hg0 1 T			g/m3	1.94E-05	19.35
C HgII 1 T			g/m3	7.24E-05	72.38
C MeHg 1 T			g/m3	1.42E-06	1.42
C Hg0 2 T			g/m3	1.29E-04	128.71
C HgII 2 T			g/m3	7.11E-04	710.83
C MeHg 2 T			g/m3	4.28E-06	4.28
C Hg0 sed			g/m3	1.07E-04	106.83
C HgII 1 sed			g/m3	1.83E+01	18331660.50
C MeHg 1 sed			g/m3	3.58E-03	3582.68
C Hg0 sed, wet			g/g	4.03E-11	0.000
C HgII 1 sed, wet			g/g	1.43E-05	14.316
C MeHg 1 sed, wet			g/g	4.29E-09	0.004
C HgT sed,wet			g/g	1.43E-05	14.320
C Hg0 sed, dry weight			g/g	2.37E-10	0.00
C HgII 1 sed, dry weight			g/g	4.07E-05	40.69
C MeHg 1 sed, dry weight			g/g	7.95E-09	0.01
C HgT 1			g/m3	9.31E-05	93.14
C HgT 2			g/m3	8.44E-04	843.82
C HgT Sed			g/g	4.07E-05	40.70

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg T/HgT)	1.52%	77.70%	20.78%
Layer 2		0.51%	84.24%	15.25%
Sediments		0.02%	99.98%	0.00%

Q'	Bulk Exchange Flow		m3/yr	3,017,619
Qin	Inflow		m3/yr	3,474,314
Qout	Outflow		m3/yr	3,474,314
Aw	Surface Area of the Water Body		m2	378,381
E	Exchange rate		m2/yr	2
V 1	Volume of Layer 1	Aw*z 1	m3	183,741
V 2	Volume of Layer 2	Aw*z 2	m3	37,838
z1	depth of first water layer		m	0.49
z2	depth of second water layer		m	0.10

f aq Hg0 w 1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f aq HgII w 1	aqueous phase fraction of HgII in water column, layer 1	0.63276%
f aq MeHg w 1	aqueous phase fraction of MeHg in water column, layer 1	8.86115%
f aq Hg0 w 2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f aq HgII w 2	aqueous phase fraction of HgII in water column, layer 2	5.59528%
f aq MeHg w 2	aqueous phase fraction of MeHg in water column, layer 2	16.16173%
f DOC Hg0 w 1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f DOC Hg0 w 2	DOC complexed fraction of HgII in water column, layer 1	3.05171%
f DOC HgII w 1	DOC complexed fraction of MeHg in water column, layer 1	43.95131%
f DOC HgII w 2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f DOC MeHg w 1	DOC complexed fraction of HgII in water column, layer 2	26.98508%
f DOC MeHg w 2	DOC complexed fraction of MeHg in water column, layer 2	80.16218%
f abio Hg0 w 1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f abio HgII w 1	abiotic particulate phase fraction of HgII in water column, layer 1	0.38210%
f abio MeHg w 1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01183%
f abio Hg0 w 2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f abio HgII w 2	abiotic particulate phase fraction of HgII in water column, layer 2	5.01537%
f abio MeHg w 2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03204%

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{d C^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{d C^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{d C^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{d C^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{d C^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{d C^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{d C^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{d C^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{d C^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9	b
C Hg0 1 T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01
C HgII 1 T	1.12E+08	-6.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01
C MeHg 1 T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01
C Hg0 2 T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	4.82E-01	-4.40E+03	0.00E+00

Matrix

C Hg0 1 T	1.935E-05	-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	1.9E-05
C HgII 1 T	7.238E-05	-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	7.2E-05
C MeHg 1 T	1.415E-06	-1.97E-16	-3.86E-16	-1.54E-07	1.96E-15	-5.89E-16	-1.43E-07	2.72E-13	6.88E-08	-1.43E-07	1.4E-06
C Hg0 2 T	1.287E-04	-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	0.00013
C HgII 2 T	7.108E-04	-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.00071
C MeHg 2 T	4.283E-06	-3.476E-16	-7.619E-16	-1.715E-07	6.42E-15	-1.91E-15	-4.65E-07	8.86E-13	2.24E-07	-4.65E-07	4.3E-06
C Hg0 sed	1.068E-04	-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	0.00011
C HgII 1 sed	1.833E+01	1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	18.3317
C MeHg 1 sed	3.583E-03	1.97E-14	-1.41E-13	-6.31E-05	6.48E-12	-5.53E-13	-1.71E-04	7.59E-10	1.92E-04	-3.98E-04	0.00358

Inverted Matrix

x=b/A

A*x=b

C T sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}\left(1 - \theta_{sed}\right)} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[\frac{10^6\ cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.94994%
L_T,Hg0	Total Load, Hg0		g/yr	3.99E-01
L_T,HgII	Total Load, HgII		g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg		g/yr	7.43E-01
Rate Constants				
kw_v,Hg0	water column volatilization loss rate constant, Hg0		per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII		per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg		per yr	1.87
kw_oxid_1	water column oxidation rate constant		per yr	610.22
kw_oxid_2	water column oxidation rate constant		per yr	525.60
kw_red_1	water column reduction rate constant, layer 2		per yr	246.95
kw_red_2	water column reduction rate constant, layer 2		per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1		per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2		per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1		per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2		per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1		per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2		per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant		per yr	0.00
kb_oxid	benthic oxidation rate constant		per yr	0.00
kb_red	benthic reduction rate constant		per yr	0.00
kb_methy	benthic methylation rate constant		per yr	0.00
kb_demeth	benthic demethylation rate constant		per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant		per yr	0.00
v_sA	abiotic settling velocity		m/yr	4792.628412
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	1.65
TSS+2			mg/L	0.21
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2		L/kg	1.59E+07
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.43E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	1.80E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-8.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}} \Big/ \frac{C_{dss,i}^{j} + C_{DOC,i}^{j}}{} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS} \Big/ C_{filtered,i}^{j}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.84E-06	4.84
C_HgII_1_Aq			g/m3	6.71E-07	0.67
C_MeHg_1_Aq			g/m3	2.40E-07	0.24
C_Hg0_2_Aq			g/m3	3.07E-05	30.71
C_HgII_2_Aq			g/m3	5.52E-05	55.20
C_MeHg_2_Aq			g/m3	1.11E-06	1.11
C_Hg0_pore			g/m3	3.07E-05	30.71
C_HgII_pore			g/m3	5.21E-05	52.09
C_MeHg_pore			g/m3	5.44E-07	0.54
C_HgT_1_filtered			g/m3	5.75E-06	5.75
C_HgT_2_filtered			g/m3	8.70E-05	87.02
C_HgT_Sed_filtered			g/m3	8.33E-05	83.34
C_Hg0_1_T			g/m3	4.84E-06	4.84
C_HgII_1_T			g/m3	1.82E-05	18.21
C_MeHg_1_T			g/m3	4.54E-07	0.45
C_Hg0_2_T			g/m3	3.07E-05	30.71
C_HgII_2_T			g/m3	1.69E-04	169.43
C_MeHg_2_T			g/m3	1.15E-06	1.15
C_Hg0_sed			g/m3	2.55E-05	25.49
C_HgII_1_sed			g/m3	4.37E+00	4,366,651.04
C_MeHg_1_sed			g/m3	9.01E-04	901.35
C_Hg0_sed, wet			g/g	9.62E-12	0.00
C_HgII_1_sed, wet			g/g	3.41E-06	3.41
C_MeHg_1_sed, wet			g/g	1.08E-09	0.00
C_HgT_sed,wet			g/g	3.41E-06	3.41
C_Hg0_sed, dry weight			g/g	5.66E-11	0.00
C_HgII_1_sed, dry weight			g/g	9.69E-06	9.69
C_MeHg_1_sed, dry weight			g/g	2.00E-09	0.00
C_HgT_1			g/m3	2.35E-05	23.50
C_HgT_2			g/m3	2.01E-04	201.28
C_HgT_Sed, dry weight			g/g	9.69E-06	9.69
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		1.93%	77.46%	20.61%
Layer 2			0.57%	84.17%	15.26%
Sediments			0.02%	99.98%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			3.05171%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			26.98508%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{oMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{met2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed
	1	2	3	4	5	6	7	8	9
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_HgII_1_T	1.12E+08	-8.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_MeHg_1_T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	4.82E-01	-4.40E+03

A*x=b

Matrix b	Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	4.844E-06	-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	4.8E-06
C_HgII_1_T	1.821E-05	-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	1.8E-05
C_MeHg_1_T	4.543E-07	-1.97E-16	-3.86E-16	-1.54E-07	1.96E-15	-5.89E-16	-1.43E-07	2.72E-13	6.88E-08	-1.43E-07	4.5E-07
C_Hg0_2_T	3.071E-05	-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	3.1E-05
C_HgII_2_T	1.694E-04	-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.00017
C_MeHg_2_T	1.151E-06	-3.476E-16	-7.619E-16	-1.715E-07	6.42E-15	-1.91E-15	-4.65E-07	8.86E-13	2.24E-07	-4.65E-07	1.2E-06
C_Hg0_sed	2.549E-05	-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	2.5E-05
C_HgII_1_sed	4.367E+00	1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	4.36665
C_MeHg_1_sed	9.014E-04	1.97E-14	-1.41E-13	-6.31E-05	6.48E-12	-5.53E-13	-1.71E-04	7.59E-10	1.92E-04	-3.98E-04	0.0009

Target C_sed, wet 4.367577874 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	388.36
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	246.95
kw_red_2	water column reduction rate constant	per yr	107.40
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for	per yr	6.43
kw_mer	water column *mer* cleavage demethy	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeH(	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	1.65
TSS+2		mg/L	0.21
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \quad \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{}{C_{dissi}^j + C_{DOC,i}^j} \quad \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = (D_{dry,i} + D_{wet,i}) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05171%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			26.98508%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.38210%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.01537%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01183%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			10.10022%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			80.80179%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			5.03141%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			62.40427%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			1.42443%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.94994%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.06
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.09
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	548.69
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1	TSS_1	1.65	mg/L	
Sbio_zoo,1	0.5	TSS_2	0.21	mg/L	
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	6.23E-02				
Sbio_dead,2	8.73E-02				
S_abio, sed	5.28E+04				
S_bio_dead,sed	5.49E+02				
S_sed,total	5.34E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			Solution	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b		Matrix							
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	2.01E+06	S_bio_dead,1	6.23E-02	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.062268
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	8.73E-02	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.08734
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	5.49E+02	0	0	0.000273	-2.50E-04	0	-3.07E-04	548.6925

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

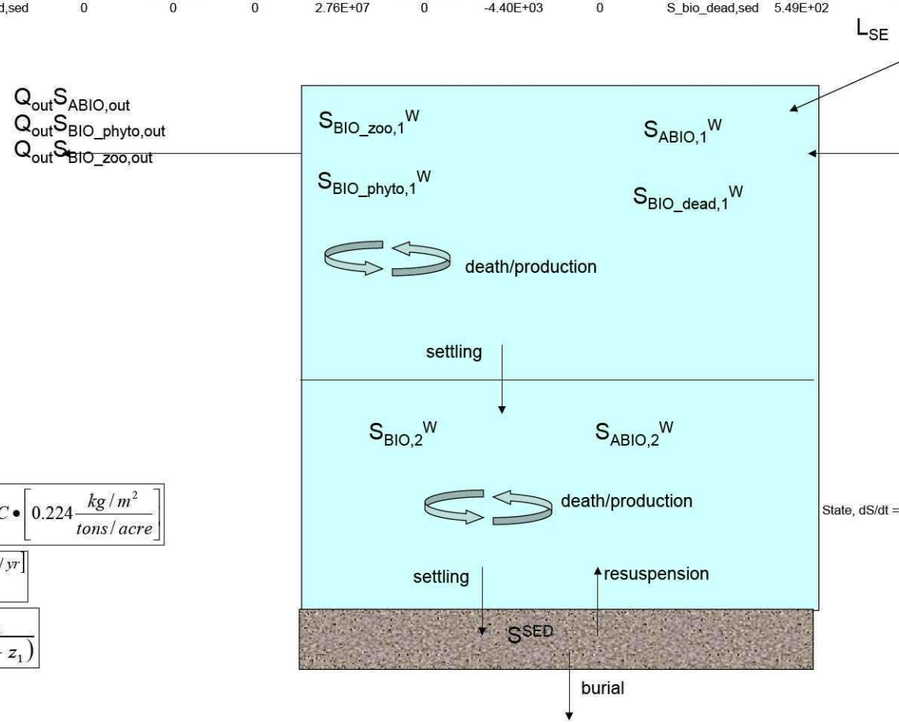
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00633	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.05595		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03052		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.26985		
k_meth_1	abiotic methylation in layer 1		per yr	2.69E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.38E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			6.33E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.60E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			2.70E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	1.56E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.38E-05	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43* ,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Little Blue Heron

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations					
Hg0	0	g/m3			
HgII	5.64E-06	g/m3	5.64	63.07894647	
MeHg	7.33E-08	g/m3	0.07332	79.56391716	Fish
Total Mercury Concentration in Contaminated Sediment, dry weight	40.7	ug/g			
Known Mercury in Contaminated Soils					
Cs,Hg0	0	g/m3	7		
Cs,HgII	1.129080624	g/m3			
Cs,MeHg	4.13E-03	g/m3			
Required Hazard Index for Sensitive Indicator	1				

Kd_abio		
HgII	7,182,936	1
MeHg	15,887	1
Kd_bio		
HgII	127,696,640	1
MeHg	2,581,565	1
Kd_DOC		
HgII	301,427	1
MeHg	310,000	1
	PCT ERROR	CLEANUP
MeHg Filtered	3.02	6.69
HgT Filtered	-32.97	
MeHg Unfilte	96.44	
HgT Unfiltere	185.83	

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	19.35	ng/L		-19.35	-100	0.47	ng/L	3.44	ng/L
	HgII Filtered	2.67	ng/L		-2.67	-100	0.07	ng/L	0.48	ng/L
	MeHg Filtered	0.75	ng/L	0.77	0.02	3.0229168	0.09	ng/L	0.19	ng/L
	HgT Filtered	22.77	ng/L	15.26	-7.51	-32.96994	0.63	ng/L	4.11	ng/L
	Hg0 Unfiltered	19.35	ng/L		-19.35	-100	0.47	ng/L	3.44	ng/L
	HgII Unfiltered	72.38	ng/L		-72.38	-100	1.89	ng/L	12.96	ng/L
	MeHg Unfiltered	1.42	ng/L	2.78	1.36	96.437458	0.16	ng/L	0.36	ng/L
	HgT Unfiltered	93.14	ng/L	266.23	173.09	185.82535	2.53	ng/L	16.76	ng/L
Hypolimnion	Hg0 Filtered	128.71	ng/L		-128.71	-100	1.20	ng/L	21.22	ng/L
	HgII Filtered	231.59	ng/L		-231.59	-100	2.08	ng/L	38.13	ng/L
	MeHg Filtered	4.13	ng/L		-4.13	-100	0.20	ng/L	0.82	ng/L
	HgT Filtered	364.42	ng/L		-364.42	-100	3.47	ng/L	60.16	ng/L
	Hg0 Unfiltered	128.71	ng/L		-128.71	-100	1.20	ng/L	21.22	ng/L
	HgII Unfiltered	710.83	ng/L		-710.83	-100	6.37	ng/L	117.02	ng/L
	MeHg Unfiltered	4.28	ng/L		-4.28	-100	0.21	ng/L	0.85	ng/L
	HgT Unfiltered	843.82	ng/L		-843.82	-100	7.77	ng/L	139.09	ng/L
	Sediment									
	Hg0 porewater	128.71	ng/L		-128.71	-100	1.20	ng/L	21.223	ng/L
	HgII porewater	218.67	ng/L		-218.67	-100	1.92	ng/L	35.963	ng/L
	MeHg porewater	2.16	ng/L		-2.16	-100	0.06	ng/L	0.387	ng/L
	HgT porewater	349.54	ng/L		-349.54	-100	3.17	ng/L	57.573	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.69	ug/g		-40.69	-100	0.19	ug/g	6.69	ug/g
	MeHg bulk, dry	0.00795	ug/g	0.00658	0.00	-17.26047	0.00	ug/g	0.00	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.357	ug/g	6.69	ug/g
	Trophic Level 3	0.68	ug/g		-0.68	-100	0.080	ug/g	0.17	ug/g
	Trophic Level 4	1.49	ug/g		-1.49	-100	0.173	ug/g	0.38	ug/g
	HI	3.92					0.46		1.00	
	Sensitive Indicator	Little Blue Heron					Little Blue Heron		Little Blue Heron	
	Target C_sed, dry	6.69	ug/g	Note: 8						
	Target C_sed, wet	3.02	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.16E-07	per day	1.16E-04
	Hypolimnion	1.16E-06	per day	
	Sediment	1.16E-07	per day	
Demethylation	Epilimnion	1.16E-08	per day	
	Hypolimnion	1.16E-07	per day	
	Sediment	2.33E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

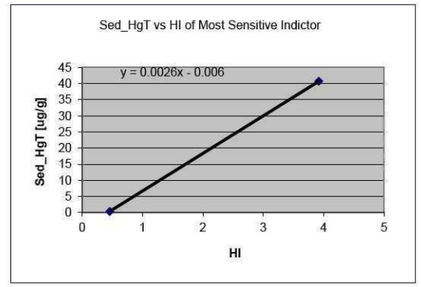
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.84	0.10	0.21
Otter	0.90	0.10	0.23
Mink	**1.75**	0.20	0.45
Great Blue Heron	**3.40**	0.40	0.87
Little Blue Heron	**3.92**	0.46	**1.00**
Pied-bill Grebe	**1.60**	0.19	0.41
Kingfisher	0.00	0.00	0.00
Wood Duck	0.62	0.07	0.16
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
3.92	40.70
0.46	0.36
m =	11.659
b=	-4.965
Sed_HgT	6.694
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under tools. Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.75	0.09	0.191	ng/L

Biota

Trophic Level 1: Phytoplankton	0.14	0.02	0.04	ug Hg/ g wet weight
Trophic Level 2: Insects	0.12	0.01	0.03	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.13	0.02	0.03	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.68	0.08	0.17	ug Hg/ g wet weight
Trophic Level 4: Bass	1.49	0.17	0.38	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.81	0.09	0.21	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.14	0.02	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.13	0.02	0.03	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Body Weight	Ingestion Rate	Drinking rate	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants	Percent of Diet from Trophic Level 2 : Insects	Percent of Diet from Trophic Level 2 : Crayfish or Frogs	Percent of Diet from Trophic Level 3 : Fish	Percent of Diet from Trophic Level 4 : Fish	Percent of Diet from nonaquatic sources	Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Insects	Potential Dose from Trophic Level 2: Crayfish	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
Animal	[kg in wet weight]	[kg wet weight/d]	[L/d]	--	--	--	--	--	--	[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	63	0	0	0	63	75	0.84
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	2	51	15	67	75	0.90
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	6	5	120	131	75	**1.75**
Great Blue Heron	2.2	0.509	0.1	0%	5%	10%	50%	35%	0%	0	0	1	3	79	120	204	60	**3.40**
Little Blue Heron	0.34	0.147	0.16	0%	25%	0%	75%	0%	0%	0	0	13	0	222	0	235	60	**3.92**
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	30	11	55	0	96	60	**1.60**
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	29	9	0	0	0	37	60	0.62
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	1	2	11	14	5000	0.00
Human																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.014	0.00	7.31	0.00	0.00	0.00	7	75	0.10
0.007	0.00	0.00	0.23	5.91	1.72	8	75	0.10
0.009	0.00	0.00	0.74	0.54	14.01	15	75	0.20
0.004	0.00	0.17	0.36	9.21	14.04	24	60	0.40
0.041	0.00	1.57	0.00	25.82	0.00	27	60	0.46
0.006	0.00	3.52	1.26	6.42	0.00	11	60	0.19
0.010	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.006	3.36	0.99	0.00	0.00	0.00	4	60	0.07
0.000	0.00	0.00	0.09	0.22	1.33	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.031	0.00	16.02	0.00	0.00	0.00	16	75	0.21
0.016	0.00	0.00	0.51	12.96	3.76	17	75	0.23
0.019	0.00	0.00	1.62	1.17	30.69	33	75	0.45
0.009	0.00	0.37	0.79	20.18	30.75	52	60	0.87
0.090	0.00	3.44	0.00	56.56	0.00	60	60	**1.00**
0.014	0.00	7.70	2.77	14.05	0.00	25	60	0.41
0.022	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.013	7.37	2.17	0.00	0.00	0.00	10	60	0.16
0.000	0.00	0.00	0.19	0.47	2.91	4	5000	0.00
							RfD	
0.003	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893.2	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.75E-07	0.47
C_HgII_1_Aq			g/m3	6.96E-08	0.07
C_MeHg_1_Aq			g/m3	8.71E-08	0.09
C_Hg0_2_Aq			g/m3	1.20E-06	1.20
C_HgII_2_Aq			g/m3	2.08E-06	2.08
C_MeHg_2_Aq			g/m3	2.00E-07	0.20
C_Hg0_pore			g/m3	1.20E-06	1.20
C_HgII_pore			g/m3	1.92E-06	1.92
C_MeHg_pore			g/m3	5.66E-08	0.06
C_HgT_1_filtered			g/m3	6.31E-07	0.63
C_HgT_2_filtered			g/m3	3.47E-06	3.47
C_HgT_Sed_filtered			g/m3	3.17E-06	3.17
C_Hg0_1_T			g/m3	4.75E-07	0.47
C_HgII_1_T			g/m3	1.89E-06	1.89
C_MeHg_1_T			g/m3	1.65E-07	0.16
C_Hg0_2_T			g/m3	1.20E-06	1.20
C_HgII_2_T			g/m3	6.37E-06	6.37
C_MeHg_2_T			g/m3	2.07E-07	0.21
C_Hg0_sed, bulk			g/m3	9.92E-07	1
C_HgII_1_sed, bulk			g/m3	1.61E-01	160,828
C_MeHg_1_sed, bulk			g/m3	9.38E-05	94
C_Hg0_sed, wet			g/g	7.75E-13	0.000
C_HgII_1_sed, wet			g/g	1.93E-07	0.193
C_MeHg_1_sed, wet			g/g	8.52E-15	0.000
C_HgT_sed,wet			g/g	1.93E-07	0.193
C_Hg0_sed, dry weight			g/g	2.20E-12	0.0000
C_HgII_1_sed, dry weight			g/g	3.57E-07	0.3570
C_MeHg_1_sed, dry weight			g/g	2.08E-10	0.0002
C_HgT_1			g/m3	2.53E-06	2.530
C_HgT_2			g/m3	7.77E-06	7.773
C_HgT_Sed, dry weight			g/g	3.57E-07	0.357
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		6.52%	74.72%	18.76%
Layer 2			2.66%	81.96%	15.37%
Sediments			0.06%	99.94%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth,2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	1.12E+08	-6.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.08E+08	0.00E+00	0.00E+00	-4.29E+03	9.64E-01
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	4.82E-01	-4.40E+03

Matrix b

C Hg0 1 T	4.746E-07
C HgII 1 T	1.890E-06
C MeHg 1 T	1.649E-07
C Hg0 2 T	1.195E-06
C HgII 2 T	6.371E-06
C MeHg 2 T	2.071E-07
C Hg0 sed	9.919E-07
C HgII 1 sed	1.608E-01
C MeHg 1 sed	9.382E-05

Solution Inverted Matrix

-1.21E-08	-1.13E-08	-4.94E-09	-1.15E-08	-1.14E-08	-5.43E-09	-1.15E-08	-1.14E-08	-5.43E-09
-2.73E-08	-4.52E-08	-1.18E-08	-4.04E-08	-4.24E-08	-1.39E-08	-4.04E-08	-4.24E-08	-1.39E-08
-1.66E-10	-2.64E-10	-1.54E-07	-6.61E-10	-7.36E-10	-1.43E-07	-6.61E-10	-7.52E-10	-1.43E-07
-1.859E-08	-2.847E-08	-1.157E-08	-1.13E-07	-7.67E-08	-1.91E-08	-1.13E-07	-7.67E-08	-1.91E-08
-9.578E-08	-1.520E-07	-5.127E-08	-3.81E-07	-4.24E-07	-7.59E-08	-3.81E-07	-4.24E-07	-7.60E-08
-5.423E-10	-8.609E-10	-1.718E-07	-2.16E-09	-2.40E-09	-4.66E-07	-2.16E-09	-2.45E-09	-4.66E-07
-1.54E-08	-2.36E-08	-9.60E-09	-9.36E-08	-6.37E-08	-1.59E-08	-4.01E-06	-6.37E-08	-1.59E-08
-2.42E-03	-3.84E-03	-1.29E-03	-9.61E-03	-1.07E-02	-1.92E-03	-9.61E-03	-1.09E-02	-1.92E-03
-4.64E-07	-7.37E-07	-6.33E-05	-1.84E-06	-2.05E-06	-1.72E-04	-1.84E-06	-2.10E-06	-3.99E-04

x=b/A

4.74599E-07	
1.89003E-06	
1.64944E-07	
1.19505E-06	
6.37108E-06	
2.07147E-07	
9.91889E-07	
0.16082824	
9.38187E-05	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.006
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.089
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.056
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.162
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.031
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.440
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.270
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.802

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.004
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.050
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.101
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.229
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.808
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.229
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.050
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.014
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.624
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.036
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		9.90E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		5.01E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		9.99E-01
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	11351.43
TSS_1		mg/L	1.65
TSS+2		mg/L	0.21
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \cdot \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.94E-05	19.35
C_HgII_1_Aq			g/m3	2.67E-06	2.67
C_MeHg_1_Aq			g/m3	7.47E-07	0.75
C_Hg0_2_Aq			g/m3	1.29E-04	128.71
C_HgII_2_Aq			g/m3	2.32E-04	231.59
C_MeHg_2_Aq			g/m3	4.13E-06	4.13
C_Hg0_pore			g/m3	1.29E-04	128.71
C_HgII_pore			g/m3	2.19E-04	218.67
C_MeHg_pore			g/m3	2.16E-06	2.16
C_HgT_1_filtered			g/m3	2.28E-05	22.77
C_HgT_2_filtered			g/m3	3.64E-04	364.42
C_HgT_Sed_filtered			g/m3	3.50E-04	349.54
C_Hg0_1_T			g/m3	1.94E-05	19.35
C_HgII_1_T			g/m3	7.24E-05	72.38
C_MeHg_1_T			g/m3	1.42E-06	1.42
C_Hg0_2_T			g/m3	1.29E-04	128.71
C_HgII_2_T			g/m3	7.11E-04	710.83
C_MeHg_2_T			g/m3	4.28E-06	4.28
C_Hg0_sed			g/m3	1.07E-04	106.83
C_HgII_1_sed			g/m3	1.83E+01	18331660.50
C_MeHg_1_sed			g/m3	3.58E-03	3582.68
C_Hg0_sed, wet			g/g	4.03E-11	0.000
C_HgII_1_sed, wet			g/g	1.43E-05	14.316
C_MeHg_1_sed, wet			g/g	4.29E-09	0.004
C_HgT_sed,wet			g/g	1.43E-05	14.320
C_Hg0_sed, dry weight			g/g	2.37E-10	0.00
C_HgII_1_sed, dry weight			g/g	4.07E-05	40.69
C_MeHg_1_sed, dry weight			g/g	7.95E-09	0.01
C_HgT_1			g/m3	9.31E-05	93.14
C_HgT_2			g/m3	8.44E-04	843.82
C_HgT_Sed			g/g	4.07E-05	40.70
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		1.52%	77.70%	20.78%
Layer 2			0.51%	84.24%	15.25%
Sediments			0.02%	99.98%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1				100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1				0.63276%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1				8.86115%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2				100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2				5.59528%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2				16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1				0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1				3.05171%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1				43.95131%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2				0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2				26.98508%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2				80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1				0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1				0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1				0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2				0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2				5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2				0.03204%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T
C_HgII_1_T	1.12E+08	-6.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	4.82E-01	-4.40E+03	0.00E+00	C_MeHg_1_sed

Solution	Inverted Matrix											x=b/A
Matrix												
1.935E-05	-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	1.94E-05		
7.238E-05	-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	7.24E-05		
1.415E-06	-1.97E-16	-3.86E-16	-1.54E-07	1.96E-15	-5.89E-16	-1.43E-07	2.72E-13	6.88E-08	-1.43E-07	1.42E-06		
1.287E-04	-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	0.000129		
7.108E-04	-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.000711		
4.283E-06	-3.476E-16	-7.619E-16	-1.715E-07	6.42E-15	-1.91E-15	-4.65E-07	8.86E-13	2.24E-07	-4.65E-07	4.28E-06		
1.068E-04	-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	0.000107		
1.833E+01	1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	18.33166		
3.583E-03	1.97E-14	-1.41E-13	-6.31E-05	6.48E-12	-5.53E-13	-1.71E-04	7.59E-10	1.92E-04	-3.98E-04	0.003583		

A*x=b

C T sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq\_i}^{sw,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

v_sA	abiotic settling velocity		m/yr	4792.628412
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	1.65
TSS+2			mg/L	0.21

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

Effective Partition Coefficients for each Hg species and layer

K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for HgII in layer 1	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for HgII in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Little Blue Heron

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	3.44E-06	3.44
C_HgII_1_Aq			g/m3	4.78E-07	0.48
C_MeHg_1_Aq			g/m3	1.91E-07	0.19
C_Hg0_2_Aq			g/m3	2.12E-05	21.22
C_HgII_2_Aq			g/m3	3.81E-05	38.13
C_MeHg_2_Aq			g/m3	8.16E-07	0.82
C_Hg0_pore			g/m3	2.12E-05	21.22
C_HgII_pore			g/m3	3.60E-05	35.96
C_MeHg_pore			g/m3	3.87E-07	0.39
C_HgT_1_filtered			g/m3	4.11E-06	4.11
C_HgT_2_filtered			g/m3	6.02E-05	60.16
C_HgT_Sed_filtered			g/m3	5.76E-05	57.57
C_Hg0_1_T			g/m3	3.44E-06	3.44
C_HgII_1_T			g/m3	1.30E-05	12.96
C_MeHg_1_T			g/m3	3.61E-07	0.36
C_Hg0_2_T			g/m3	2.12E-05	21.22
C_HgII_2_T			g/m3	1.17E-04	117.02
C_MeHg_2_T			g/m3	8.47E-07	0.85
C_Hg0_sed			g/m3	1.76E-05	17.62
C_HgII_1_sed			g/m3	3.01E+00	3,014,880.33
C_MeHg_1_sed			g/m3	6.42E-04	641.81
C_Hg0_sed, wet			g/g	6.65E-12	0.00
C_HgII_1_sed, wet			g/g	2.35E-06	2.35
C_MeHg_1_sed, wet			g/g	7.69E-10	0.00
C_HgT_sed,wet			g/g	2.36E-06	2.36
C_Hg0_sed, dry weight			g/g	3.91E-11	0.00
C_HgII_1_sed, dry weight			g/g	6.69E-06	6.69
C_MeHg_1_sed, dry weight			g/g	1.42E-09	0.00
C_HgT_1			g/m3	1.68E-05	16.76
C_HgT_2			g/m3	1.39E-04	139.09
C_HgT_Sed, dry weight			g/g	6.69E-06	6.69
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		2.16%	77.32%	20.52%
Layer 2			0.61%	84.13%	15.26%
Sediments			0.02%	99.98%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			3.05171%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			26.98508%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{Hg1,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{s,B} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{Hg1,1}}{dt} = L_{T,Hg1,1} + Q_{in} C_{in,Hg1,1} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg1,1} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg1,1} A_w - v_{s,B} \cdot f^{w,1}_{bioHg1,1} A_w\right] \cdot C^w_{Hg1,1} + Q' \cdot C^w_{Hg1,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{Hg1,1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s,A} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{s,B} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{Hg1,2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{Hg1,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioHg1,1} A_w - v_{s,B} \cdot f^{w,2}_{bioHg1,1} A_w - R_{sw} \cdot f^{w,2}_{aqHg1}\right] \cdot C^w_{Hg1,2} + Q' \cdot C^w_{Hg1,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg1}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg1,1} A_w\right] \cdot C^{sed}_{aqHg1}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{Hg1,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,A} \cdot f^{w,2}_{abioHg0} + v_{s,B} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,A} \cdot f^{w,2}_{abioHgII} + v_{s,B} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,A} \cdot f^{w,2}_{abioMeHg} + v_{s,B} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed	Matrix		Solution Matrix	Inverted Matrix									x=b/A
	1	2	3	4	5	6	7	8	9	b												
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	3.440E-06	-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	3.4E-06
C_HgII_1_T	1.12E+08	-8.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.296E-05	-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	1.3E-05
C_MeHg_1_T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	3.613E-07	-1.97E-16	-3.86E-16	-1.54E-07	1.96E-15	-5.89E-16	-1.43E-07	2.72E-13	6.88E-08	-1.43E-07	3.6E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	2.122E-05	-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	2.1E-05
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	1.170E-04	-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.00012
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00	C_MeHg_2_T	8.473E-07	-3.476E-16	-7.619E-16	-1.715E-07	6.42E-15	-1.91E-15	-4.65E-07	8.86E-13	2.24E-07	-4.65E-07	8.5E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	1.762E-05	-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	1.8E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	3.02E+00	C_HgII_1_sed	3.015E+00	1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	3.01488
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	4.82E-01	-4.40E+03	0.00E+00	C_MeHg_1_sed	6.418E-04	1.97E-14	-1.41E-13	-6.31E-05	6.48E-12	-5.53E-13	-1.71E-04	7.59E-10	1.92E-04	-3.98E-04	0.00064

A*x=b

Target C_sed, wet 3.015539747 g/g

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Little Blue Heron

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	388.36
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	246.95
kw_red_2	water column reduction rate constant	per yr	107.40
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for	per yr	6.43
kw_mer	water column *mer* cleavage demethy	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeH(	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	1.65
TSS+2		mg/L	0.21
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{sw,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \quad \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{}{C_{dizz,i}^j + C_{DOC,i}^j} = \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = (D_{dry,i} + D_{wet,i}) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w} \right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2} \right) Sc_{w,i}^{-0.67} \left(3.15 x 10^{7} \right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log\left(\mu_w\right) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2} \right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = \left(1.32 + 0.009 \bullet T_a\right) x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05171%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			26.98508%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.38210%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.01537%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01183%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			10.10022%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			80.80179%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			5.03141%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			62.40427%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			1.42443%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.94994%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.06
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.09
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	548.69
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1		TSS_1	1.65	mg/L
Sbio_zoo,1	0.5		TSS_2	0.21	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	6.23E-02				
Sbio_dead,2	8.73E-02				
S_abio, sed	5.28E+04				
S_bio_dead,sed	5.49E+02				
S_sed,total	5.34E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			Solution	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b		Matrix							
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	2.01E+06	S_bio_dead,1	6.23E-02	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.062268
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	8.73E-02	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.08734
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	5.49E+02	0	0	0.000273	-2.50E-04	0	-3.07E-04	548.6925

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

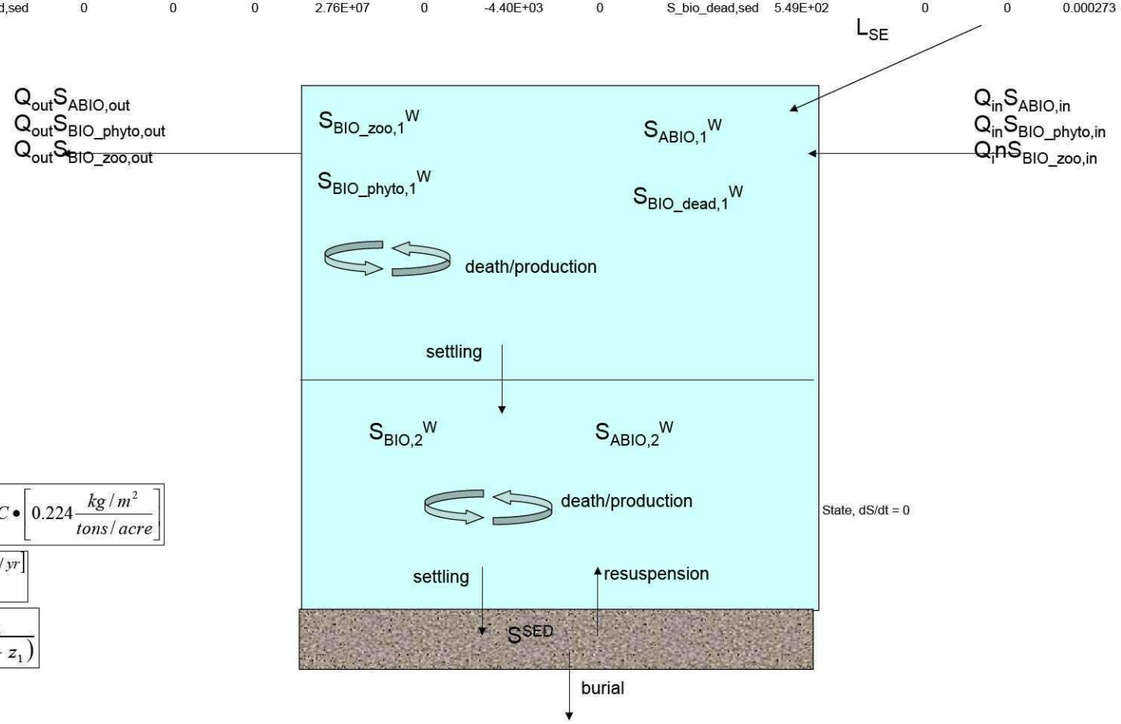
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East	
A		kg/m2/yr	0.2016		
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200		12
K	Soil Erodibility Factor	(kg/km2)	0.3		
LS	Topographic Factor	--	2.5		
C	Cover Management Factor	--	0.006		

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)	50-300	250-1000	>1000	<50-500
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00633	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.05595		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03052		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.26985		
k_meth_1	abiotic methylation in layer 1		per yr	2.69E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.38E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			6.33E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.60E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			2.70E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	1.56E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.38E-05	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weatl		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Great Blue Heron

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations			
Hg0	0	g/m3	
HgII	5.64E-06	g/m3	5.64
MeHg	7.33E-08	g/m3	0.07332

Total Mercury Concentration in Contaminated Sediment, dry weight	40.7	ug/g

Known Mercury in Contaminated Soils			
Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio		
HgII	7,182,936	1
MeHg	15,887	1

Kd_bio		
HgII	127,696,640	1
MeHg	2,581,565	1

Kd_DOC		
HgII	301,427	1
MeHg	310,000	1

	PCT ERROR	CLEANUP
MeHg Filtered	3.02	8.46
HgT Filtered	-32.97	
MeHg Unfilte	96.44	
HgT Unfiltere	185.83	

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	19.35	ng/L		-19.35	-100	0.47	ng/L	4.27	ng/L
	HgII Filtered	2.67	ng/L		-2.67	-100	0.07	ng/L	0.59	ng/L
	MeHg Filtered	0.75	ng/L	0.77	0.02	3.0229168	0.09	ng/L	0.22	ng/L
	HgT Filtered	22.77	ng/L	15.26	-7.51	-32.96994	0.63	ng/L	5.08	ng/L
	Hg0 Unfiltered	19.35	ng/L		-19.35	-100	0.47	ng/L	4.27	ng/L
	HgII Unfiltered	72.38	ng/L		-72.38	-100	1.89	ng/L	16.05	ng/L
	MeHg Unfiltered	1.42	ng/L	2.78	1.36	96.437458	0.16	ng/L	0.42	ng/L
	HgT Unfiltered	93.14	ng/L	266.23	173.09	185.82535	2.53	ng/L	20.74	ng/L
Hypolimnion	Hg0 Filtered	128.71	ng/L		-128.71	-100	1.20	ng/L	26.82	ng/L
	HgII Filtered	231.59	ng/L		-231.59	-100	2.08	ng/L	48.20	ng/L
	MeHg Filtered	4.13	ng/L		-4.13	-100	0.20	ng/L	0.99	ng/L
	HgT Filtered	364.42	ng/L		-364.42	-100	3.47	ng/L	76.01	ng/L
	Hg0 Unfiltered	128.71	ng/L		-128.71	-100	1.20	ng/L	26.82	ng/L
	HgII Unfiltered	710.83	ng/L		-710.83	-100	6.37	ng/L	147.94	ng/L
	MeHg Unfiltered	4.28	ng/L		-4.28	-100	0.21	ng/L	1.03	ng/L
	HgT Unfiltered	843.82	ng/L		-843.82	-100	7.77	ng/L	175.78	ng/L
	Sediment									
	Hg0 porewater	128.71	ng/L		-128.71	-100	1.20	ng/L	26.819	ng/L
	HgII porewater	218.67	ng/L		-218.67	-100	1.92	ng/L	45.476	ng/L
	MeHg porewater	2.16	ng/L		-2.16	-100	0.06	ng/L	0.479	ng/L
	HgT porewater	349.54	ng/L		-349.54	-100	3.17	ng/L	72.774	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.69	ug/g		-40.69	-100	0.19	ug/g	8.46	ug/g
	MeHg bulk, dry	0.00795	ug/g	0.00658	0.00	-17.26047	0.00	ug/g	0.00	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.357	ug/g	8.46	ug/g
Fish	Trophic Level 3	0.68	ug/g		-0.68	-100	0.080	ug/g	0.20	ug/g
	Trophic Level 4	1.49	ug/g		-1.49	-100	0.173	ug/g	0.44	ug/g
	HI	3.40					0.40		1.00	
	Sensitive Indicator	Great Blue Heron					Great Blue Heron		Great Blue Heron	
	Target C_sed, dry	8.46	ug/g	Note: 8						
	Target C_sed, wet	3.81	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.16E-07	per day	1.16E-04
	Hypolimnion	1.16E-06	per day	
	Sediment	1.16E-07	per day	
Demethylation	Epilimnion	1.16E-08	per day	
	Hypolimnion	1.16E-07	per day	
	Sediment	2.33E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

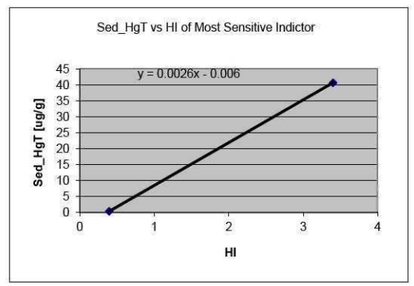
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed
Wildlife			Target-Level
Little Brown Bat	0.84	0.10	0.25
Otter	0.90	0.10	0.26
Mink	**1.75**	0.20	0.51
Great Blue Heron	**3.40**	0.40	**1.00**
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	**1.60**	0.19	0.47
Kingfisher	0.00	0.00	0.00
Wood Duck	0.62	0.07	0.18
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
3.40	40.70
0.40	0.36
m =	13.429
b=	-4.965
Sed_HgT	8.464
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under tools. Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

	Site-Specific User Input	Required
	Model Calculated	No input required
	Data Necessary for certain sites	Only necessary if applicable to site of interest
	Scenario 1 Output	
	Scenario 2 Output	
	Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.75	0.09	0.220	ng/L

Biota

Trophic Level 1: Phytoplankton	0.14	0.02	0.04	ug Hg/ g wet weight
Trophic Level 2: Insects	0.12	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.13	0.02	0.04	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.68	0.08	0.20	ug Hg/ g wet weight
Trophic Level 4: Bass	1.49	0.17	0.44	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.81	0.09	0.24	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.14	0.02	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.13	0.02	0.04	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

Wildlife Specific Parameters

Animal	Body Weight [kg in wet weight]	Ingestion Rate [kg wet weight/d]	Drinking rate [L/d]	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants --	Percent of Diet from Trophic Level 2 : Insects --	Percent of Diet from Trophic Level 2 : Crayfish or Frogs --	Percent of Diet from Trophic Level 3 : Fish --	Percent of Diet from Trophic Level 4 : Fish --	Percent of Diet from nonaquatic sources --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%
Great Blue Heron	2.2	0.509	0.1	0%	5%	10%	50%	35%	0%
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%

Contaminated Sediment Calculations

Animal	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0	0	63	0	0	0	63	75	0.84
Otter	0	0	0	2	51	15	67	75	0.90
Mink	0	0	0	6	5	120	131	75	**1.75**
Great Blue Heron	0	0	1	3	79	120	204	60	**3.40**
Little Blue Heron	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0	0	30	11	55	0	96	60	**1.60**
Kingfisher	0	0	0	0	0	0	0	60	0.00
Wood Duck	0	29	9	0	0	0	37	60	0.62
Alligator	0	0	0	1	2	11	14	5000	0.00

Human

Human Specific Parameters

Human																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution 5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.014	0.00	7.31	0.00	0.00	0.00	7	75	0.10
0.007	0.00	0.00	0.23	5.91	1.72	8	75	0.10
0.009	0.00	0.00	0.74	0.54	14.01	15	75	0.20
0.004	0.00	0.17	0.36	9.21	14.04	24	60	0.40
0.041	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.006	0.00	3.52	1.26	6.42	0.00	11	60	0.19
0.010	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.006	3.36	0.99	0.00	0.00	0.00	4	60	0.07
0.000	0.00	0.00	0.09	0.22	1.33	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.035	0.00	18.45	0.00	0.00	0.00	18	75	0.25
0.018	0.00	0.00	0.59	14.92	4.33	20	75	0.26
0.022	0.00	0.00	1.87	1.35	35.35	39	75	0.51
0.010	0.00	0.42	0.92	23.24	35.42	60	60	**1.00**
0.103	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.016	0.00	8.87	3.19	16.19	0.00	28	60	0.47
0.025	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.015	8.49	2.50	0.00	0.00	0.00	11	60	0.18
0.000	0.00	0.00	0.22	0.55	3.35	4	5000	0.00
							RfD	
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil	Kd-suspended matter	Kd-sediment	DOC/Water	multiplier for Kd_abio to Kd_bio	Kd-bio	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
						L/kg	L/kg	L/kg	L/kg		L/kg		
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893.2	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.38

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.75E-07	0.47
C_HgII_1_Aq			g/m3	6.96E-08	0.07
C_MeHg_1_Aq			g/m3	8.71E-08	0.09
C_Hg0_2_Aq			g/m3	1.20E-06	1.20
C_HgII_2_Aq			g/m3	2.08E-06	2.08
C_MeHg_2_Aq			g/m3	2.00E-07	0.20
C_Hg0_pore			g/m3	1.20E-06	1.20
C_HgII_pore			g/m3	1.92E-06	1.92
C_MeHg_pore			g/m3	5.66E-08	0.06
C_HgT_1_filtered			g/m3	6.31E-07	0.63
C_HgT_2_filtered			g/m3	3.47E-06	3.47
C_HgT_Sed_filtered			g/m3	3.17E-06	3.17
C_Hg0_1_T			g/m3	4.75E-07	0.47
C_HgII_1_T			g/m3	1.89E-06	1.89
C_MeHg_1_T			g/m3	1.65E-07	0.16
C_Hg0_2_T			g/m3	1.20E-06	1.20
C_HgII_2_T			g/m3	6.37E-06	6.37
C_MeHg_2_T			g/m3	2.07E-07	0.21
C_Hg0_sed, bulk			g/m3	9.92E-07	1
C_HgII_1_sed, bulk			g/m3	1.61E-01	160,828
C_MeHg_1_sed, bulk			g/m3	9.38E-05	94
C_Hg0_sed, wet			g/g	7.75E-13	0.000
C_HgII_1_sed, wet			g/g	1.93E-07	0.193
C_MeHg_1_sed, wet			g/g	8.52E-15	0.000
C_HgT_sed,wet			g/g	1.93E-07	0.193
C_Hg0_sed, dry weight			g/g	2.20E-12	0.0000
C_HgII_1_sed, dry weight			g/g	3.57E-07	0.3570
C_MeHg_1_sed, dry weight			g/g	2.08E-10	0.0002
C_HgT_1			g/m3	2.53E-06	2.530
C_HgT_2			g/m3	7.77E-06	7.773
C_HgT_Sed, dry weight			g/g	3.57E-07	0.357
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		6.52%	74.72%	18.76%
Layer 2			2.66%	81.96%	15.37%
Sediments			0.06%	99.94%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth,2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9
C Hg0 1 T	**-1.90E+08**	**4.54E+07**	**2.39E+06**	**3.02E+06**	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	**1.12E+08**	**-6.02E+07**	**2.88E-02**	0.00E+00	**3.02E+06**	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	**4.94E-02**	**-9.84E+06**	0.00E+00	0.00E+00	**3.02E+06**	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	**3.018E+06**	0.000E+00	0.000E+00	**-2.31E+07**	**4.06E+06**	**2.43E+05**	**2.55E+05**	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	**1.134E+07**	0.000E+00	**1.99E+07**	**-1.15E+08**	**5.24E-01**	0.00E+00	**4.29E+03**	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	**3.626E+06**	0.00E+00	**5.24E-01**	**-4.88E+06**	0.00E+00	0.00E+00	**4.40E+03**
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	**2.12E+05**	0.00E+00	0.00E+00	**-2.55E+05**	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	**1.08E+08**	0.00E+00	0.00E+00	**-4.29E+03**	**9.64E-01**
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	**1.62E+06**	0.00E+00	**4.82E-01**	**-4.40E+03**

b

C Hg0 1 T	**-3.99E-01**
C HgII 1 T	**-4.13E+01**
C MeHg 1 T	**-9.97E-01**
C Hg0 2 T	0.00E+00
C HgII 2 T	0.00E+00
C MeHg 2 T	0.00E+00
C Hg0 sed	0.00E+00
C HgII 1 sed	0.00E+00
C MeHg 1 sed	0.00E+00

Matrix

C Hg0 1 T	4.746E-07
C HgII 1 T	1.890E-06
C MeHg 1 T	1.649E-07
C Hg0 2 T	1.195E-06
C HgII 2 T	6.371E-06
C MeHg 2 T	2.071E-07
C Hg0 sed	9.919E-07
C HgII 1 sed	1.608E-01
C MeHg 1 sed	9.382E-05

Solution Inverted Matrix

-1.21E-08	**-1.13E-08**	**-4.94E-09**	**-1.15E-08**	**-1.14E-08**	**-5.43E-09**	**-1.15E-08**	**-1.14E-08**	**-5.43E-09**	4.74599E-07
-2.73E-08	**-4.52E-08**	**-1.18E-08**	**-4.04E-08**	**-4.24E-08**	**-1.39E-08**	**-4.04E-08**	**-4.24E-08**	**-1.39E-08**	1.89003E-06
-1.66E-10	**-2.64E-10**	**-1.54E-07**	**-6.61E-10**	**-7.36E-10**	**-1.43E-07**	**-6.61E-10**	**-7.52E-10**	**-1.43E-07**	1.64944E-07
-1.859E-08	**-2.847E-08**	**-1.157E-08**	**-1.13E-07**	**-7.67E-08**	**-1.91E-08**	**-1.13E-07**	**-7.67E-08**	**-1.91E-08**	1.19505E-06
-9.578E-08	**-1.520E-07**	**-5.127E-08**	**-3.81E-07**	**-4.24E-07**	**-7.59E-08**	**-3.81E-07**	**-4.24E-07**	**-7.60E-08**	6.37108E-06
-5.423E-10	**-8.609E-10**	**-1.718E-07**	**-2.16E-09**	**-2.40E-09**	**-4.66E-07**	**-2.16E-09**	**-2.45E-09**	**-4.66E-07**	2.07147E-07
-1.54E-08	**-2.36E-08**	**-9.60E-09**	**-9.36E-08**	**-6.37E-08**	**-1.59E-08**	**-4.01E-06**	**-6.37E-08**	**-1.59E-08**	9.91889E-07
-2.42E-03	**-3.84E-03**	**-1.29E-03**	**-9.61E-03**	**-1.07E-02**	**-1.92E-03**	**-9.61E-03**	**-1.09E-02**	**-1.92E-03**	0.16082824
-4.64E-07	**-7.37E-07**	**-6.33E-05**	**-1.84E-06**	**-2.05E-06**	**-1.72E-04**	**-1.84E-06**	**-2.10E-06**	**-3.99E-04**	9.38187E-05

x=b/A

Symbol	Parameter	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.006
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.089
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.056
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.162
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.031
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.440
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.270
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.802

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.004
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			0.050
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			0.101
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			0.229
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			0.808
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			0.229
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			0.050
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			0.014
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			0.624
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			0.036
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			9.90E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			5.01E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			9.99E-01
L_T,Hg0	Total Load, Hg0		g/yr	3.99E-01
L_T,HgII	Total Load, HgII		g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg		g/yr	7.43E-01
Rate Constants				
kw_v,Hg0	water column volatilization loss rate constant, Hg0		per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII		per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg		per yr	1.87
kw_oxid_1	water column oxidation rate constant		per yr	610.22
kw_oxid_2	water column oxidation rate constant		per yr	525.60
kw_red_1	water column reduction rate constant, layer 2		per yr	246.95
kw_red_2	water column reduction rate constant, layer 2		per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1		per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2		per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1		per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2		per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1		per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2		per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant		per yr	0.00
kb_oxid	benthic oxidation rate constant		per yr	0.00
kb_red	benthic reduction rate constant		per yr	0.00
kb_methy	benthic methylation rate constant		per yr	0.00
kb_demeth	benthic demethylation rate constant		per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant		per yr	0.00
v_sA	abiotic settling velocity		m/yr	4,792.63
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.030
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	1.65
TSS+2			mg/L	0.21
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1		L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2		L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2		L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	1.80E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \cdot \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.94E-05	19.35
C_HgII_1_Aq			g/m3	2.67E-06	2.67
C_MeHg_1_Aq			g/m3	7.47E-07	0.75
C_Hg0_2_Aq			g/m3	1.29E-04	128.71
C_HgII_2_Aq			g/m3	2.32E-04	231.59
C_MeHg_2_Aq			g/m3	4.13E-06	4.13
C_Hg0_pore			g/m3	1.29E-04	128.71
C_HgII_pore			g/m3	2.19E-04	218.67
C_MeHg_pore			g/m3	2.16E-06	2.16
C_HgT_1_filtered			g/m3	2.28E-05	22.77
C_HgT_2_filtered			g/m3	3.64E-04	364.42
C_HgT_Sed_filtered			g/m3	3.50E-04	349.54
C_Hg0_1_T			g/m3	1.94E-05	19.35
C_HgII_1_T			g/m3	7.24E-05	72.38
C_MeHg_1_T			g/m3	1.42E-06	1.42
C_Hg0_2_T			g/m3	1.29E-04	128.71
C_HgII_2_T			g/m3	7.11E-04	710.83
C_MeHg_2_T			g/m3	4.28E-06	4.28
C_Hg0_sed			g/m3	1.07E-04	106.83
C_HgII_1_sed			g/m3	1.83E+01	18331660.50
C_MeHg_1_sed			g/m3	3.58E-03	3582.68
C_Hg0_sed, wet			g/g	4.03E-11	0.000
C_HgII_1_sed, wet			g/g	1.43E-05	14.316
C_MeHg_1_sed, wet			g/g	4.29E-09	0.004
C_HgT_sed,wet			g/g	1.43E-05	14.320
C_Hg0_sed, dry weight			g/g	2.37E-10	0.00
C_HgII_1_sed, dry weight			g/g	4.07E-05	40.69
C_MeHg_1_sed, dry weight			g/g	7.95E-09	0.01
C_HgT_1			g/m3	9.31E-05	93.14
C_HgT_2			g/m3	8.44E-04	843.82
C_HgT_Sed			g/g	4.07E-05	40.70
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		1.52%	77.70%	20.78%
Layer 2			0.51%	84.24%	15.25%
Sediments			0.02%	99.98%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1				100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1				0.63276%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1				8.86115%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2				100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2				5.59528%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2				16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1				0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1				3.05171%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1				43.95131%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2				0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2				26.98508%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2				80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1				0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1				0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1				0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2				0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2				5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2				0.03204%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{ox1} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T
C_HgII_1_T	1.12E+08	-6.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	4.82E-01	-4.40E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix											x=b/A
1.935E-05	-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	1.94E-05	C_Hg0_1_T	19.35
7.238E-05	-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	7.24E-05	C_HgII_1_T	72.38
1.415E-06	-1.97E-16	-3.86E-16	-1.54E-07	1.96E-15	-5.89E-16	-1.43E-07	2.72E-13	6.88E-08	-1.43E-07	1.42E-06	C_MeHg_1_T	1.42
1.287E-04	-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	0.000129	C_Hg0_2_T	128.71
7.108E-04	-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.000711	C_HgII_2_T	710.83
4.283E-06	-3.476E-16	-7.619E-16	-1.715E-07	6.42E-15	-1.91E-15	-4.65E-07	8.86E-13	2.24E-07	-4.65E-07	4.28E-06	C_MeHg_2_T	4.28
1.068E-04	-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	0.000107	C_Hg0_sed	106.83
1.833E+01	1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	18.33166	C_HgII_1_sed	18331660.50
3.583E-03	1.97E-14	-1.41E-13	-6.31E-05	6.48E-12	-5.53E-13	-1.71E-04	7.59E-10	1.92E-04	-3.98E-04	0.003583	C_MeHg_1_sed	3582.68

A*x=b

C T sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\ \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq\_i}^{sw,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	1.65
TSS+2			mg/L	0.21
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2		L/kg	1.59E+07
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.43E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	1.80E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.27E-06	4.27
C_HgII_1_Aq			g/m3	5.92E-07	0.59
C_MeHg_1_Aq			g/m3	2.20E-07	0.22
C_Hg0_2_Aq			g/m3	2.68E-05	26.82
C_HgII_2_Aq			g/m3	4.82E-05	48.20
C_MeHg_2_Aq			g/m3	9.88E-07	0.99
C_Hg0_pore			g/m3	2.68E-05	26.82
C_HgII_pore			g/m3	4.55E-05	45.48
C_MeHg_pore			g/m3	4.79E-07	0.48
C_HgT_1_filtered			g/m3	5.08E-06	5.08
C_HgT_2_filtered			g/m3	7.60E-05	76.01
C_HgT_Sed_filtered			g/m3	7.28E-05	72.77
C_Hg0_1_T			g/m3	4.27E-06	4.27
C_HgII_1_T			g/m3	1.61E-05	16.05
C_MeHg_1_T			g/m3	4.16E-07	0.42
C_Hg0_2_T			g/m3	2.68E-05	26.82
C_HgII_2_T			g/m3	1.48E-04	147.94
C_MeHg_2_T			g/m3	1.03E-06	1.03
C_Hg0_sed			g/m3	2.23E-05	22.26
C_HgII_1_sed			g/m3	3.81E+00	3,812,354.77
C_MeHg_1_sed			g/m3	7.95E-04	794.92
C_Hg0_sed, wet			g/g	8.40E-12	0.00
C_HgII_1_sed, wet			g/g	2.98E-06	2.98
C_MeHg_1_sed, wet			g/g	9.52E-10	0.00
C_HgT_sed,wet			g/g	2.98E-06	2.98
C_Hg0_sed, dry weight			g/g	4.94E-11	0.00
C_HgII_1_sed, dry weight			g/g	8.46E-06	8.46
C_MeHg_1_sed, dry weight			g/g	1.76E-09	0.00
C_HgT_1			g/m3	2.07E-05	20.74
C_HgT_2			g/m3	1.76E-04	175.78
C_HgT_Sed, dry weight			g/g	8.46E-06	8.46
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		2.01%	77.41%	20.58%
Layer 2			0.58%	84.16%	15.26%
Sediments			0.02%	99.98%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			3.05171%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			26.98508%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{s,B} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHgII} A_w - v_{s,B} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s,A} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{s,B} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot A_w \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioHgII} A_w - v_{s,B} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,A} \cdot f^{w,2}_{abioHg0} + v_{s,B} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,A} \cdot f^{w,2}_{abioHgII} + v_{s,B} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,A} \cdot f^{w,2}_{abioMeHg} + v_{s,B} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed	Matrix b		Solution Matrix
	1	2	3	4	5	6	7	8	9	b		
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	4.268E-06
C_HgII_1_T	1.12E+08	-8.02E+07	2.88E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.605E-05
C_MeHg_1_T	0.00E+00	4.94E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	4.162E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	2.682E-05
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	5.24E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	1.479E-04
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	5.24E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00	C_MeHg_2_T	1.026E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	2.226E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	3.81E+00	C_HgII_1_sed	3.812E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	4.82E-01	-4.40E+03	0.00E+00	C_MeHg_1_sed

Inverted Matrix

-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	4.3E-06
-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	1.6E-05
-1.97E-16	-3.86E-16	-1.54E-07	1.96E-15	-5.89E-16	-1.43E-07	2.72E-13	6.88E-08	-1.43E-07	4.2E-07
-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	2.7E-05
-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.00015
-3.476E-16	-7.619E-16	-1.715E-07	6.42E-15	-1.91E-15	-4.65E-07	8.86E-13	2.24E-07	-4.65E-07	1E-06
-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	2.2E-05
1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	3.81235
1.97E-14	-1.41E-13	-6.31E-05	6.48E-12	-5.53E-13	-1.71E-04	7.59E-10	1.92E-04	-3.98E-04	0.00079

x=b/A

A*x=b

Target C_sed, wel 3.813171955 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	388.36
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	246.95
kw_red_2	water column reduction rate constant	per yr	107.40
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for	per yr	6.43
kw_mer	water column *mer* cleavage demethy	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeH(	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	1.65
TSS+2		mg/L	0.21
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{}{C_{diss,i}^j + C_{DOC,i}^j} \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = (D_{dry,i} + D_{wet,i}) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left(K_{L,i}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- =	Total Chloride
SO_4^{2-} =	Total Sulfate
S^{2-} =	Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05171%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			26.98508%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.38210%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.01537%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01183%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			10.10022%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			80.80179%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			5.03141%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			62.40427%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			1.42443%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.94994%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.06
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.09
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	548.69
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1	TSS_1	1.65	mg/L	
Sbio_zoo,1	0.5	TSS_2	0.21	mg/L	
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	6.23E-02				
Sbio_dead,2	8.73E-02				
S_abio, sed	5.28E+04				
S_bio_dead,sed	5.49E+02				
S_sed,total	5.34E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			Solution	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b		Matrix							
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	2.01E+06	S_bio_dead,1	6.23E-02	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.062268
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	8.73E-02	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.08734
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	5.49E+02	0	0	0.000273	-2.50E-04	0	-3.07E-04	548.6925

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

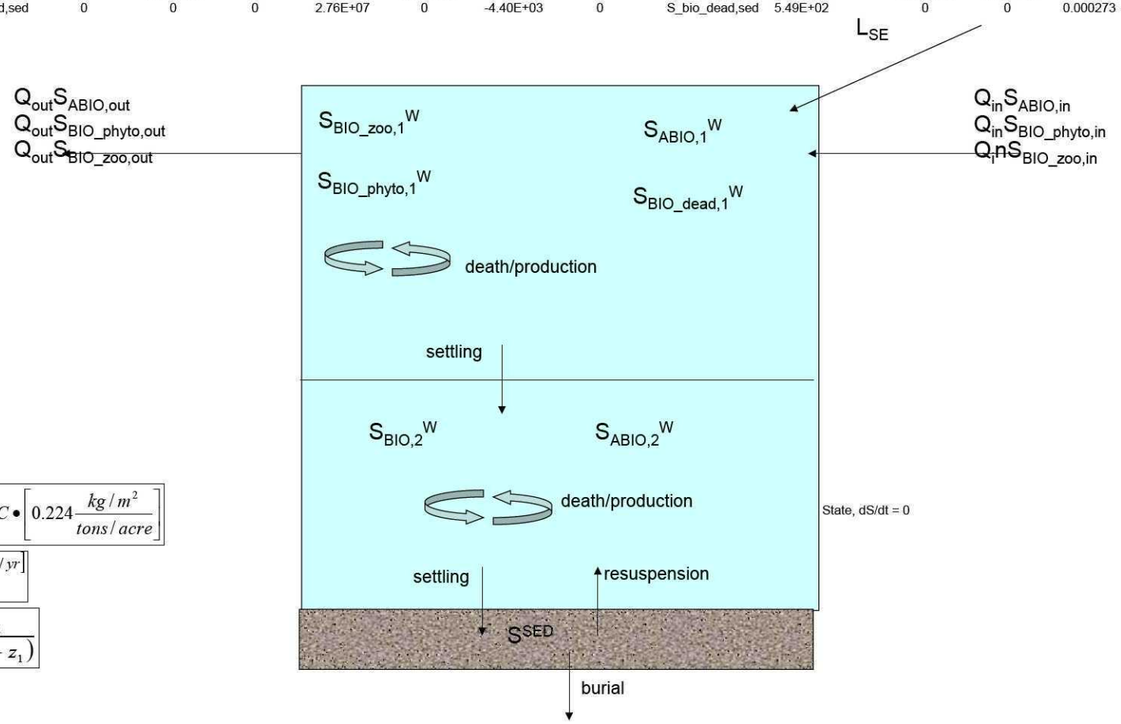
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00633	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.05595		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03052		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.26985		
k_meth_1	abiotic methylation in layer 1		per yr	2.69E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.38E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	1.16364E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	4.24727E-05		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			6.33E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.60E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			2.70E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	1.56E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.38E-05	

$$k_{demeth} = k_{demeth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	2.32727E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	8.49455E-05		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	1
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

$$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43* ,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Pied-Billed Grebe

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	43.76620569
MeHg	7.33E-08	g/m3	0.07332	72.01444878
Total Mercury Concentration in Contaminated Sediment, dry weight	40.7	ug/g		
Known Mercury in Contaminated Soils				
Cs,Hg0	0	g/m3	7	
Cs,HgII	1.129080624	g/m3		
Cs,MeHg	4.13E-03	g/m3		
Required Hazard Index for Sensitive Indicator	1			

Exposure Concentrations

Kd_abio			
HgII	7,182,936	1	
MeHg	15,887	1	
Kd_bio			
HgII	127,696,640	1	
MeHg	2,581,565	1	
Kd_DOC			
HgII	301,427	1	
MeHg	310,000	1	
	PCT ERROR	CLEANUP	
MeHg Filtered	-22.77	15.38	
HgT Filtered	-33.73		
MeHg Unfilter	47.26		
HgT Unfiltere	184.30		

			Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered		19.36	ng/L		-19.36	-100	0.47	ng/L	7.51	ng/L
	HgII Filtered		2.67	ng/L		-2.67	-100	0.07	ng/L	1.04	ng/L
	MeHg Filtered		1.00	ng/L	0.77	-0.23	-22.76904	0.09	ng/L	0.43	ng/L
	HgT Filtered		23.03	ng/L	15.26	-7.77	-33.72745	0.63	ng/L	8.97	ng/L
	Hg0 Unfiltered		19.36	ng/L		-19.36	-100	0.47	ng/L	7.51	ng/L
	HgII Unfiltered		72.39	ng/L		-72.39	-100	1.89	ng/L	28.15	ng/L
	MeHg Unfiltered		1.89	ng/L	2.78	0.89	47.259026	0.17	ng/L	0.81	ng/L
	HgT Unfiltered		93.64	ng/L	266.23	172.59	184.30228	2.53	ng/L	36.47	ng/L
Hypolimnion	Hg0 Filtered		128.72	ng/L		-128.72	-100	1.19	ng/L	48.69	ng/L
	HgII Filtered		231.58	ng/L		-231.58	-100	2.07	ng/L	87.56	ng/L
	MeHg Filtered		5.61	ng/L		-5.61	-100	0.21	ng/L	2.22	ng/L
	HgT Filtered		365.90	ng/L		-365.90	-100	3.48	ng/L	138.47	ng/L
	Hg0 Unfiltered		128.72	ng/L		-128.72	-100	1.19	ng/L	48.69	ng/L
	HgII Unfiltered		710.78	ng/L		-710.78	-100	6.36	ng/L	268.75	ng/L
	MeHg Unfiltered		5.82	ng/L		-5.82	-100	0.22	ng/L	2.31	ng/L
	HgT Unfiltered		845.32	ng/L		-845.32	-100	7.77	ng/L	319.75	ng/L
	Sediment										
	Hg0 porewater		128.72	ng/L		-128.72	-100	1.19	ng/L	48.693	ng/L
	HgII porewater		218.65	ng/L		-218.65	-100	1.92	ng/L	82.646	ng/L
	MeHg porewater		2.96	ng/L		-2.96	-100	0.06	ng/L	1.141	ng/L
	HgT porewater		350.33	ng/L		-350.33	-100	3.17	ng/L	132.480	ng/L
	Hg0 bulk, dry		0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry		40.69	ug/g		-40.69	-100	0.19	ug/g	15.38	ug/g
	MeHg bulk, dry		0.01088	ug/g	0.00658	0.00	-39.5231	0.00	ug/g	0.00	ug/g
	HgT bulk, dry		40.70	ug/g	40.7	0.00	0	0.357	ug/g	15.38	ug/g
	Trophic Level 3	Fish	0.91	ug/g		-0.91	-100	0.082	ug/g	0.39	ug/g
	Trophic Level 4		1.98	ug/g		-1.98	-100	0.178	ug/g	0.85	ug/g
	HI		2.33					0.21		1.00	
	Sensitive Indicator		Mink					Mink		Mink	
	Target C_sed, dry		15.38	ug/g	Note: 8						
	Target C_sed, wet		6.93	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.60E-07	per day	1.60E-04
	Hypolimnion	1.60E-06	per day	
	Sediment	1.60E-07	per day	
Demethylation	Epilimnion	1.60E-08	per day	
	Hypolimnion	1.60E-07	per day	
	Sediment	3.20E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

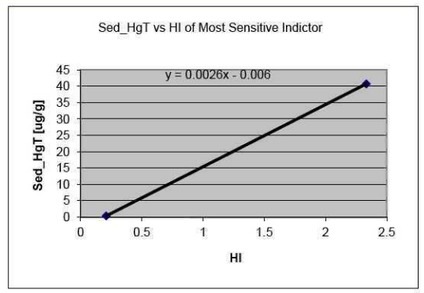
Human and Wildlife Exposure Risk Results

6,250

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	1.12	0.10	0.48
Otter	1.20	0.11	0.51
Mink	**2.33**	0.21	**1.00**
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	**2.14**	0.19	0.92
Kingfisher	0.00	0.00	0.00
Wood Duck	0.83	0.07	0.36
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
2.33	40.70
0.21	0.36
m =	18.995
b=	-3.612
Sed_HgT	15.384
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	1.00	0.09	0.427	ng/L

Biota

Trophic Level 1: Phytoplankton	0.19	0.02	0.08	ug Hg/ g wet weight
Trophic Level 2: Insects	0.17	0.01	0.07	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.18	0.02	0.08	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.91	0.08	0.39	ug Hg/ g wet weight
Trophic Level 4: Bass	1.98	0.18	0.85	ug Hg/ g wet weight
Trophic Level 3: Silverside	1.08	0.10	0.46	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.19	0.02	0.08	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.17	0.02	0.07	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

Wildlife Specific Parameters

Animal	Body Weight [kg in wet weight]	Ingestion Rate [kg wet weight/d]	Drinking rate [L/d]	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants --	Percent of Diet from Trophic Level 2 : Insects --	Percent of Diet from Trophic Level 2 : Crayfish or Frogs --	Percent of Diet from Trophic Level 3 : Fish --	Percent of Diet from Trophic Level 4 : Fish --	Percent of Diet from nonaquatic sources --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%

Contaminated Sediment Calculations

Animal	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0	0	84	0	0	0	84	75	1.12
Otter	0	0	0	3	68	20	90	75	1.20
Mink	0	0	0	8	6	160	175	75	2.33
Great Blue Heron	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0	0	40	14	73	0	128	60	2.14
Kingfisher	0	0	0	0	0	0	0	60	0.00
Wood Duck	0	39	11	0	0	0	50	60	0.83
Alligator	0	0	0	1	2	15	19	5000	0.00

Human

Human Specific Parameters

																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution 5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.014	0.00	7.50	0.00	0.00	0.00	7	75	0.10
0.007	0.00	0.00	0.24	6.06	1.76	8	75	0.11
0.009	0.00	0.00	0.76	0.55	14.36	16	75	0.21
0.004	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.042	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.006	0.00	3.60	1.29	6.58	0.00	11	60	0.19
0.010	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.006	3.45	1.02	0.00	0.00	0.00	4	60	0.07
0.000	0.00	0.00	0.09	0.22	1.36	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.068	0.00	35.88	0.00	0.00	0.00	36	75	0.48
0.036	0.00	0.00	1.14	29.02	8.42	39	75	0.51
0.043	0.00	0.00	3.63	2.63	68.74	75	75	**1.00**
0.019	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.201	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.031	0.00	17.25	6.20	31.48	0.00	55	60	0.92
0.048	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.029	16.51	4.86	0.00	0.00	0.00	21	60	0.36
0.000	0.00	0.00	0.43	1.06	6.52	8	5000	0.00
							RfD	
0.008	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Pied-Billed Grebe

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes			Oligo	Meso	Eutro	Dystro	
1	Trophic Status is determined DOC in Epiliminon as:		<3	3-5	5-10	10+	mg DOC/L
	from Wetzel	Flag	1	2	3	4	
2	Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.74E-07	0.47
C_HgII_1_Aq			g/m3	6.96E-08	0.07
C_MeHg_1_Aq			g/m3	8.93E-08	0.09
C_Hg0_2_Aq			g/m3	1.19E-06	1.19
C_HgII_2_Aq			g/m3	2.07E-06	2.07
C_MeHg_2_Aq			g/m3	2.12E-07	0.21
C_Hg0_pore			g/m3	1.19E-06	1.19
C_HgII_pore			g/m3	1.92E-06	1.92
C_MeHg_pore			g/m3	6.35E-08	0.06
C_HgT_1_filtered			g/m3	6.33E-07	0.63
C_HgT_2_filtered			g/m3	3.48E-06	3.48
C_HgT_Sed_filtered			g/m3	3.17E-06	3.17
C_Hg0_1_T			g/m3	4.74E-07	0.47
C_HgII_1_T			g/m3	1.89E-06	1.89
C_MeHg_1_T			g/m3	1.69E-07	0.17
C_Hg0_2_T			g/m3	1.19E-06	1.19
C_HgII_2_T			g/m3	6.36E-06	6.36
C_MeHg_2_T			g/m3	2.21E-07	0.22
C_Hg0_sed, bulk			g/m3	9.91E-07	1
C_HgII_1_sed, bulk			g/m3	1.61E-01	160,567
C_MeHg_1_sed, bulk			g/m3	1.05E-04	105
C_Hg0_sed, wet			g/g	7.74E-13	0.000
C_HgII_1_sed, wet			g/g	1.92E-07	0.192
C_MeHg_1_sed, wet			g/g	9.56E-15	0.000
C_HgT_sed,wet			g/g	1.92E-07	0.192
C_Hg0_sed, dry weight			g/g	2.20E-12	0.0000
C_HgII_1_sed, dry weight			g/g	3.56E-07	0.3564
C_MeHg_1_sed, dry weight			g/g	2.34E-10	0.0002
C_HgT_1			g/m3	2.53E-06	2.533
C_HgT_2			g/m3	7.77E-06	7.775
C_HgT_Sed, dry weight			g/g	3.57E-07	0.357
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		6.68%	74.59%	18.73%
Layer 2			2.84%	81.81%	15.35%
Sediments			0.07%	99.93%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	1.12E+08	-6.02E+07	3.95E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	6.79E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	7.20E-01	0.00E+00	4.29E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	7.20E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.08E+08	0.00E+00	0.00E+00	-4.29E+03	1.33E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	6.63E-01	-4.40E+03

b

C Hg0 1 T	4.744E-07
C HgII 1 T	1.889E-06
C MeHg 1 T	1.691E-07
C Hg0 2 T	1.193E-06
C HgII 2 T	6.361E-06
C MeHg 2 T	2.206E-07
C Hg0 sed	9.905E-07
C HgII 1 sed	1.606E-01
C MeHg 1 sed	1.053E-04

Matrix Solution — Inverted Matrix — x=b/A

C Hg0 1 T	-1.21E-08	-1.12E-08	-4.94E-09	-1.14E-08	-1.13E-08	-5.43E-09	-1.14E-08	-1.13E-08	-5.43E-09	4.74427E-07
C HgII 1 T	-2.73E-08	-4.52E-08	-1.18E-08	-4.04E-08	-4.24E-08	-1.39E-08	-4.04E-08	-4.23E-08	-1.39E-08	1.88921E-06
C MeHg 1 T	-2.28E-10	-3.62E-10	-1.54E-07	-9.07E-10	-1.01E-09	-1.43E-07	-9.07E-10	-1.03E-09	-1.43E-07	1.69063E-07
C Hg0 2 T	-1.857E-08	-2.843E-08	-1.156E-08	-1.13E-07	-7.66E-08	-1.91E-08	-1.13E-07	-7.66E-08	-1.91E-08	1.19338E-06
C HgII 2 T	-9.563E-08	-1.518E-07	-5.120E-08	-3.80E-07	-4.23E-07	-7.58E-08	-3.80E-07	-4.23E-07	-7.59E-08	6.36099E-06
C MeHg 2 T	-7.444E-10	-1.182E-09	-1.719E-07	-2.96E-09	-3.29E-09	-4.66E-07	-2.96E-09	-3.37E-09	-4.66E-07	2.20576E-07
C Hg0 sed	-1.54E-08	-2.36E-08	-9.59E-09	-9.35E-08	-6.36E-08	-1.59E-08	-4.01E-06	-6.36E-08	-1.59E-08	9.90504E-07
C HgII 1 sed	-2.41E-03	-3.83E-03	-1.29E-03	-9.59E-03	-1.07E-02	-1.91E-03	-9.59E-03	-1.09E-02	-1.92E-03	0.160566903
C MeHg 1 sed	-6.37E-07	-1.01E-06	-6.34E-05	-2.53E-06	-2.82E-06	-1.72E-04	-2.53E-06	-2.88E-06	-3.99E-04	0.000105314

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.004
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			0.050
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			0.101
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			0.229
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			0.808
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			0.229
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			0.050
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			0.014
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			0.624
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			0.036
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			9.90E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			5.01E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			9.99E-01
L_T,Hg0	Total Load, Hg0		g/yr	3.99E-01
L_T,HgII	Total Load, HgII		g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg		g/yr	7.43E-01
Rate Constants				
kw_v,Hg0	water column volatilization loss rate constant, Hg0		per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII		per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg		per yr	1.87
kw_oxid_1	water column oxidation rate constant		per yr	610.22
kw_oxid_2	water column oxidation rate constant		per yr	525.60
kw_red_1	water column reduction rate constant, layer 2		per yr	246.95
kw_red_2	water column reduction rate constant, layer 2		per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1		per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2		per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1		per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2		per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1		per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2		per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant		per yr	0.00
kb_oxid	benthic oxidation rate constant		per yr	0.00
kb_red	benthic reduction rate constant		per yr	0.00
kb_methy	benthic methylation rate constant		per yr	0.00
kb_demeth	benthic demethylation rate constant		per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant		per yr	0.00
v_sA	abiotic settling velocity		m/yr	4,792.63
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.030
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	1.65
TSS+2			mg/L	0.21
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1		L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2		L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2		L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	1.80E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \Big/ \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS} = \frac{C_{filtered,i}^{j}}{C_{diss,i}^{j}+C_{DOC,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.94E-05	19.36
C_HgII_1_Aq			g/m3	2.67E-06	2.67
C_MeHg_1_Aq			g/m3	9.97E-07	1.00
C_Hg0_2_Aq			g/m3	1.29E-04	128.72
C_HgII_2_Aq			g/m3	2.32E-04	231.58
C_MeHg_2_Aq			g/m3	5.61E-06	5.61
C_Hg0_pore			g/m3	1.29E-04	128.72
C_HgII_pore			g/m3	2.19E-04	218.65
C_MeHg_pore			g/m3	2.96E-06	2.96
C_HgT_1_filtered			g/m3	2.30E-05	23.03
C_HgT_2_filtered			g/m3	3.66E-04	365.90
C_HgT_Sed_filtered			g/m3	3.50E-04	350.33
C_Hg0_1_T			g/m3	1.94E-05	19.36
C_HgII_1_T			g/m3	7.24E-05	72.39
C_MeHg_1_T			g/m3	1.89E-06	1.89
C_Hg0_2_T			g/m3	1.29E-04	128.72
C_HgII_2_T			g/m3	7.11E-04	710.78
C_MeHg_2_T			g/m3	5.82E-06	5.82
C_Hg0_sed			g/m3	1.07E-04	106.83
C_HgII_1_sed			g/m3	1.83E+01	18330341.64
C_MeHg_1_sed			g/m3	4.90E-03	4901.52
C_Hg0_sed, wet			g/q	4.03E-11	0.000
C_HgII_1_sed, wet			g/q	1.43E-05	14.315
C_MeHg_1_sed, wet			g/q	5.87E-09	0.006
C_HgT_sed,wet			g/q	1.43E-05	14.321
C_Hg0_sed, dry weight			g/q	2.37E-10	0.00
C_HgII_1_sed, dry weight			g/q	4.07E-05	40.69
C_MeHg_1_sed, dry weight			g/q	1.09E-08	0.01
C_HgT_1			g/m3	9.36E-05	93.64
C_HgT_2			g/m3	8.45E-04	845.32
C_HgT_Sed			g/g	4.07E-05	40.70
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		2.02%	77.31%	20.68%
Layer 2			0.69%	84.08%	15.23%
Sediments			0.03%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.63276%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.86115%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	5.59528%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.05171%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	43.95131%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	26.98508%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03204%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{s2} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{s2} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{s2} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{s2} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{s2} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} A_w - v_{s2} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{s1} \cdot f^{w,2}_{abioHg0} + v_{s2} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{s1} \cdot f^{w,2}_{abioHgII} + v_{s2} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{s2} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T
C_HgII_1_T	1.12E+08	-6.02E+07	3.95E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	6.79E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	7.20E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	7.20E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	6.63E-01	-4.40E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix											x=b/A
1.936E-05	-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	1.94E-05	C_Hg0_1_T	19.36
7.239E-05	-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	7.24E-05	C_HgII_1_T	72.39
1.888E-06	-2.70E-16	-5.31E-16	-1.54E-07	2.69E-15	-8.10E-16	-1.43E-07	3.74E-13	9.46E-08	-1.43E-07	1.89E-06	C_MeHg_1_T	1.89
1.287E-04	-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	0.000129	C_Hg0_2_T	128.72
7.108E-04	-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.000711	C_HgII_2_T	710.78
5.824E-06	-4.780E-16	-1.048E-15	-1.715E-07	8.83E-15	-2.62E-15	-4.65E-07	1.22E-12	3.08E-07	-4.65E-07	5.82E-06	C_MeHg_2_T	5.82
1.068E-04	-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	0.000107	C_Hg0_sed	106.83
1.833E+01	1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	18.33034	C_HgII_1_sed	18330341.64
4.902E-03	2.70E-14	-1.94E-13	-6.31E-05	8.91E-12	-7.60E-13	-1.71E-04	1.04E-09	2.64E-04	-3.98E-04	0.004902	C_MeHg_1_sed	4901.52

A*x=b

C_T_sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{sw,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	1.65
TSS+2			mg/L	0.21
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2		L/kg	1.59E+07
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.43E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	1.80E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	7.51E-06	7.51
C_HgII_1_Aq			g/m3	1.04E-06	1.04
C_MeHg_1_Aq			g/m3	4.27E-07	0.43
C_Hg0_2_Aq			g/m3	4.87E-05	48.69
C_HgII_2_Aq			g/m3	8.76E-05	87.56
C_MeHg_2_Aq			g/m3	2.22E-06	2.22
C_Hg0_pore			g/m3	4.87E-05	48.69
C_HgII_pore			g/m3	8.26E-05	82.65
C_MeHg_pore			g/m3	1.14E-06	1.14
C_HgT_1_filtered			g/m3	8.97E-06	8.97
C_HgT_2_filtered			g/m3	1.38E-04	138.47
C_HgT_Sed_filtered			g/m3	1.32E-04	132.48
C_Hg0_1_T			g/m3	7.51E-06	7.51
C_HgII_1_T			g/m3	2.82E-05	28.15
C_MeHg_1_T			g/m3	8.09E-07	0.81
C_Hg0_2_T			g/m3	4.87E-05	48.69
C_HgII_2_T			g/m3	2.69E-04	268.75
C_MeHg_2_T			g/m3	2.31E-06	2.31
C_Hg0_sed			g/m3	4.04E-05	40.42
C_HgII_1_sed			g/m3	6.93E+00	6,928,453.97
C_MeHg_1_sed			g/m3	1.89E-03	1,891.81
C_Hg0_sed, wet			g/g	1.53E-11	0.00
C_HgII_1_sed, wet			g/g	5.41E-06	5.41
C_MeHg_1_sed, wet			g/g	2.27E-09	0.00
C_HgT_sed,wet			g/g	5.41E-06	5.41
C_Hg0_sed, dry weight			g/g	8.97E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.54E-05	15.38
C_MeHg_1_sed, dry weight			g/g	4.20E-09	0.00
C_HgT_1			g/m3	3.65E-05	36.47
C_HgT_2			g/m3	3.20E-04	319.75
C_HgT_Sed, dry weight			g/g	1.54E-05	15.38
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		2.22%	77.19%	20.59%
Layer 2			0.72%	84.05%	15.23%
Sediments			0.03%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
z2	depth of second water layer		m	0	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.63276%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.86115%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	5.59528%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.05171%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	43.95131%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	26.98508%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	80.16218%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{Hg1I} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abiaMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{Hg1I} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiaHgII} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHgII} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abiaHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abiaHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abiaMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_HgII_1_T	1.12E+08	-6.02E+07	3.95E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_MeHg_1_T	0.00E+00	6.79E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	7.20E-01	0.00E+00	4.29E+03	0.00E+00
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	7.20E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	6.63E-01	-4.40E+03

Matrix b

C_Hg0_1_T	-3.99E-01
C_HgII_1_T	-4.13E+01
C_MeHg_1_T	-9.97E-01
C_Hg0_2_T	0.00E+00
C_HgII_2_T	0.00E+00
C_MeHg_2_T	0.00E+00
C_Hg0_sed	0.00E+00
C_HgII_1_sed	6.93E+00
C_MeHg_1_sed	0.00E+00

Solution Matrix

C_Hg0_1_T	7.510E-06
C_HgII_1_T	2.815E-05
C_MeHg_1_T	8.093E-07
C_Hg0_2_T	4.869E-05
C_HgII_2_T	2.687E-04
C_MeHg_2_T	2.308E-06
C_Hg0_sed	4.042E-05
C_HgII_1_sed	6.928E+00
C_MeHg_1_sed	1.892E-03

Inverted Matrix

-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09
-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09
-2.70E-16	-5.31E-16	-1.54E-07	2.69E-15	-8.10E-16	-1.43E-07	3.74E-13	9.46E-08	-1.43E-07
-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09
-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08
-4.780E-16	-1.048E-15	-1.715E-07	8.83E-15	-2.62E-15	-4.65E-07	1.22E-12	3.08E-07	-4.65E-07
-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09
1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04
2.70E-14	-1.94E-13	-6.31E-05	8.91E-12	-7.60E-13	-1.71E-04	1.04E-09	2.64E-04	-3.98E-04

x=b/A

7.51E-06				
1.04E-06				
4.87E-05				
8.76E-05				
2.22E-06				
4.87E-05				
8.26E-05				
1.14E-06				
8.97E-06				
1.38E-04				
1.32E-04				
7.51E-06				
2.82E-05				
8.09E-07				
4.87E-05				
2.69E-04				
2.31E-06				
4.04E-05				
6.928454				
0.001892				

A*x=b

Target C_sed, wet 6.930386198 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.36210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate cc	per yr	388.36
kw_v,HgII	water column volatilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatilization loss rate cc	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	246.95
kw_red_2	water column reduction rate constant,	per yr	107.40
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for I	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for I	per yr	6.43
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	1.65
TSS+2		mg/L	0.21
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} = \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS}$$
$$\frac{}{C_{diss,i}^j + C_{DOC,i}^j} \qquad \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = (D_{dry,i} + D_{wet,i}) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w} \right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2} \right) Sc_{w,i}^{-0.67} \left(3.15 x 10^{7} \right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log\left(\mu_w\right) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2} \right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = \left(1.32 + 0.009 \bullet T_a\right) x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05171%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			26.98508%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.38210%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.01537%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01183%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			10.10022%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			80.80179%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			5.03141%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			62.40427%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			1.42443%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.94994%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.06
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.09
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	548.69
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1		TSS_1	1.65	mg/L
Sbio_zoo,1	0.5		TSS_2	0.21	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	6.23E-02				
Sbio_dead,2	8.73E-02				
S_abio, sed	5.28E+04				
S_bio_dead,sed	5.49E+02				
S_sed,total	5.34E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			Solution	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b		Matrix							
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	2.01E+06	S_bio_dead,1	6.23E-02	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.062268
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	8.73E-02	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.08734
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	5.49E+02	0	0	0.000273	-2.50E-04	0	-3.07E-04	548.6925

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

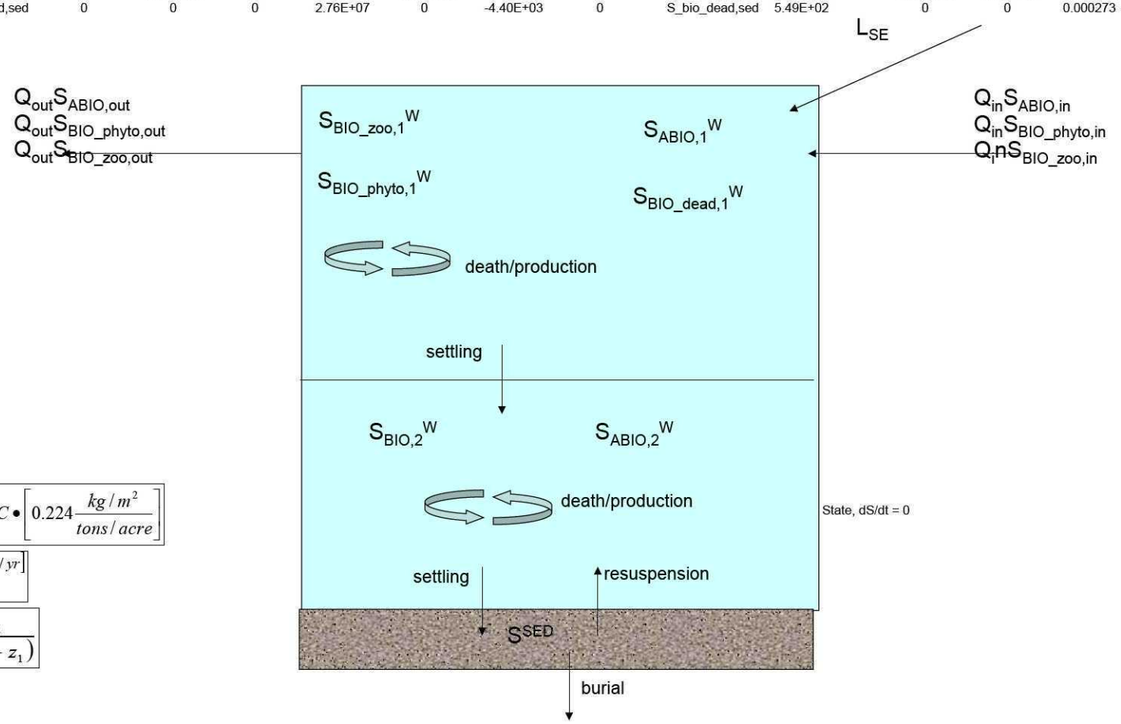
Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	0.00000016	1	2
k_meth_2	abiotic* methylation in layer 2		per day	0.0000016	1	4
k_meth_1	abiotic methylation in layer 1		per yr	0.0000584		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000584		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00633	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.05595		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03052		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.26985		
k_meth_1	abiotic methylation in layer 1		per yr	3.70E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.90E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	0.00000016	1	2
k_meth_b	biotic methylation in sediments		per yr	0.0000584		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	0.000000016	1
k_demeth_2	biotic demethylation in layer 2		per day	0.00000016	
k_demeth_1	biotic demethylation in layer 1		per yr	0.00000584	
k_demeth_2	biotic demethylation in layer 2		per yr	0.0000584	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			6.33E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.60E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			2.70E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.15E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.90E-05	

$$k_{demeth} = k_{demeth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608. mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	0.00000032	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.0001168		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{.856}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Mink

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	43.76620569
MeHg	7.33E-08	g/m3	0.07332	72.01444878

Total Mercury Concentration in Contaminated Sediment, dry weight	40.7 ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio				
HgII	7,182,936	1		
MeHg	15,887	1		
Kd_bio				
HgII	127,696,640	1		
MeHg	2,581,565	1		
Kd_DOC				
HgII	301,427	1		
MeHg	310,000	1		
	PCT ERROR	CLEANUP		
MeHg Filtered	-22.77	15.38		
HgT Filtered	-33.73			
MeHg Unfilter	47.26			
HgT Unfiltere	184.30			

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	19.36	ng/L		-19.36	-100	0.47	ng/L	7.51	ng/L
	HgII Filtered	2.67	ng/L		-2.67	-100	0.07	ng/L	1.04	ng/L
	MeHg Filtered	1.00	ng/L	0.77	-0.23	-22.76904	0.09	ng/L	0.43	ng/L
	HgT Filtered	23.03	ng/L	15.26	-7.77	-33.72745	0.63	ng/L	8.97	ng/L
	Hg0 Unfiltered	19.36	ng/L		-19.36	-100	0.47	ng/L	7.51	ng/L
	HgII Unfiltered	72.39	ng/L		-72.39	-100	1.89	ng/L	28.15	ng/L
	MeHg Unfiltered	1.89	ng/L	2.78	0.89	47.259026	0.17	ng/L	0.81	ng/L
	HgT Unfiltered	93.64	ng/L	266.23	172.59	184.30228	2.53	ng/L	36.47	ng/L
Hypolimnion	Hg0 Filtered	128.72	ng/L		-128.72	-100	1.19	ng/L	48.69	ng/L
	HgII Filtered	231.58	ng/L		-231.58	-100	2.07	ng/L	87.56	ng/L
	MeHg Filtered	5.61	ng/L		-5.61	-100	0.21	ng/L	2.22	ng/L
	HgT Filtered	365.90	ng/L		-365.90	-100	3.48	ng/L	138.47	ng/L
	Hg0 Unfiltered	128.72	ng/L		-128.72	-100	1.19	ng/L	48.69	ng/L
	HgII Unfiltered	710.78	ng/L		-710.78	-100	6.36	ng/L	268.75	ng/L
	MeHg Unfiltered	5.82	ng/L		-5.82	-100	0.22	ng/L	2.31	ng/L
	HgT Unfiltered	845.32	ng/L		-845.32	-100	7.77	ng/L	319.75	ng/L
	Sediment									
	Hg0 porewater	128.72	ng/L		-128.72	-100	1.19	ng/L	48.693	ng/L
	HgII porewater	218.65	ng/L		-218.65	-100	1.92	ng/L	82.646	ng/L
	MeHg porewater	2.96	ng/L		-2.96	-100	0.06	ng/L	1.141	ng/L
	HgT porewater	350.33	ng/L		-350.33	-100	3.17	ng/L	132.480	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.69	ug/g		-40.69	-100	0.19	ug/g	15.38	ug/g
	MeHg bulk, dry	0.01088	ug/g	0.00658	0.00	-39.5231	0.00	ug/g	0.00	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.357	ug/g	15.38	ug/g
Fish	Trophic Level 3	0.91	ug/g		-0.91	-100	0.082	ug/g	0.39	ug/g
	Trophic Level 4	1.98	ug/g		-1.98	-100	0.178	ug/g	0.85	ug/g
	HI	2.33					0.21		1.00	
	Sensitive Indicator	Mink					Mink		Mink	
	Target C_sed, dry	15.38	ug/g	Note: 8						
	Target C_sed, wet	6.93	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.60E-07	per day	1.60E-04
	Hypolimnion	1.60E-06	per day	
	Sediment	1.60E-07	per day	
Demethylation	Epilimnion	1.60E-08	per day	
	Hypolimnion	1.60E-07	per day	
	Sediment	3.20E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

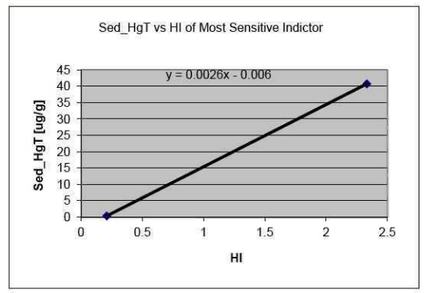
Human and Wildlife Exposure Risk Results

6,250

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	1.12	0.10	0.48
Otter	1.20	0.11	0.51
Mink	**2.33**	0.21	**1.00**
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	**2.14**	0.19	0.92
Kingfisher	0.00	0.00	0.00
Wood Duck	0.83	0.07	0.36
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
2.33	40.70
0.21	0.36
m =	18.995
b=	-3.612
Sed_HgT	15.384
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	1.00	0.09	0.427	ng/L

Biota

Trophic Level 1: Phytoplankton	0.19	0.02	0.08	ug Hg/ g wet weight
Trophic Level 2: Insects	0.17	0.01	0.07	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.18	0.02	0.08	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.91	0.08	0.39	ug Hg/ g wet weight
Trophic Level 4: Bass	1.98	0.18	0.85	ug Hg/ g wet weight
Trophic Level 3: Silverside	1.08	0.10	0.46	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.19	0.02	0.08	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.17	0.02	0.07	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Body Weight	Ingestion Rate	Drinking rate	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants	Percent of Diet from Trophic Level 2 : Insects	Percent of Diet from Trophic Level 2 : Crayfish or Frogs	Percent of Diet from Trophic Level 3 : Fish	Percent of Diet from Trophic Level 4 : Fish	Percent of Diet from nonaquatic sources	Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Insects	Potential Dose from Trophic Level 2: Crayfish	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
Animal	[kg in wet weight]	[kg wet weight/d]	[L/d]	--	--	--	--	--	--	[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	84	0	0	0	84	75	**1.12**
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	3	68	20	90	75	**1.20**
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	8	6	160	175	75	**2.33**
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	40	14	73	0	128	60	**2.14**
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	39	11	0	0	0	50	60	0.83
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	1	2	15	19	5000	0.00
Human																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.014	0.00	7.50	0.00	0.00	0.00	7	75	0.10
0.007	0.00	0.00	0.24	6.06	1.76	8	75	0.11
0.009	0.00	0.00	0.76	0.55	14.36	16	75	0.21
0.004	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.042	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.006	0.00	3.60	1.29	6.58	0.00	11	60	0.19
0.010	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.006	3.45	1.02	0.00	0.00	0.00	4	60	0.07
0.000	0.00	0.00	0.09	0.22	1.36	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.068	0.00	35.88	0.00	0.00	0.00	36	75	0.48
0.036	0.00	0.00	1.14	29.02	8.42	39	75	0.51
0.043	0.00	0.00	3.63	2.63	68.74	75	75	**1.00**
0.019	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.201	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.031	0.00	17.25	6.20	31.48	0.00	55	60	0.92
0.048	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.029	16.51	4.86	0.00	0.00	0.00	21	60	0.36
0.000	0.00	0.00	0.43	1.06	6.52	8	5000	0.00
							RfD	
0.008	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	127,696,640	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.74E-07	0.47
C_HgII_1_Aq			g/m3	6.96E-08	0.07
C_MeHg_1_Aq			g/m3	8.93E-08	0.09
C_Hg0_2_Aq			g/m3	1.19E-06	1.19
C_HgII_2_Aq			g/m3	2.07E-06	2.07
C_MeHg_2_Aq			g/m3	2.12E-07	0.21
C_Hg0_pore			g/m3	1.19E-06	1.19
C_HgII_pore			g/m3	1.92E-06	1.92
C_MeHg_pore			g/m3	6.35E-08	0.06
C_HgT_1_filtered			g/m3	6.33E-07	0.63
C_HgT_2_filtered			g/m3	3.48E-06	3.48
C_HgT_Sed_filtered			g/m3	3.17E-06	3.17
C_Hg0_1_T			g/m3	4.74E-07	0.47
C_HgII_1_T			g/m3	1.89E-06	1.89
C_MeHg_1_T			g/m3	1.69E-07	0.17
C_Hg0_2_T			g/m3	1.19E-06	1.19
C_HgII_2_T			g/m3	6.36E-06	6.36
C_MeHg_2_T			g/m3	2.21E-07	0.22
C_Hg0_sed, bulk			g/m3	9.91E-07	1
C_HgII_1_sed, bulk			g/m3	1.61E-01	160,567
C_MeHg_1_sed, bulk			g/m3	1.05E-04	105
C_Hg0_sed, wet			g/g	7.74E-13	0.000
C_HgII_1_sed, wet			g/g	1.92E-07	0.192
C_MeHg_1_sed, wet			g/g	9.56E-15	0.000
C_HgT_sed,wet			g/g	1.92E-07	0.192
C_Hg0_sed, dry weight			g/g	2.20E-12	0.0000
C_HgII_1_sed, dry weight			g/g	3.56E-07	0.3564
C_MeHg_1_sed, dry weight			g/g	2.34E-10	0.0002
C_HgT_1			g/m3	2.53E-06	2.533
C_HgT_2			g/m3	7.77E-06	7.775
C_HgT_Sed, dry weight			g/g	3.57E-07	0.357
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		6.68%	74.59%	18.73%
Layer 2			2.84%	81.81%	15.35%
Sediments			0.07%	99.93%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.006
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.089
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.056
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.162
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.031
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.440
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.270
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.802

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi}V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red,2} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,A} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,A} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,A} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	4.744E-07	-1.21E-08	-1.12E-08	-4.94E-09	-1.14E-08	-1.13E-08	-5.43E-09	-1.14E-08	-1.13E-08	-5.43E-09	4.74427E-07
C_HgII_1_T	1.12E+08	-6.02E+07	3.95E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.889E-06	-2.73E-08	-4.52E-08	-1.18E-08	-4.04E-08	-4.24E-08	-1.39E-08	-4.04E-08	-4.23E-08	-1.39E-08	1.88921E-06
C_MeHg_1_T	0.00E+00	6.79E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	1.691E-07	-2.28E-10	-3.62E-10	-1.54E-07	-9.07E-10	-1.01E-09	-1.43E-07	-9.07E-10	-1.03E-09	-1.43E-07	1.69063E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.193E-06	-1.857E-08	-2.843E-08	-1.156E-08	-1.13E-07	-7.66E-08	-1.91E-08	-1.13E-07	-7.66E-08	-1.91E-08	1.19338E-06
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	7.20E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	6.361E-06	-9.563E-08	-1.518E-07	-5.120E-08	-3.80E-07	-4.23E-07	-7.58E-08	-3.80E-07	-4.23E-07	-7.59E-08	6.36099E-06
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	7.20E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00	C_MeHg_2_T	2.206E-07	-7.444E-10	-1.182E-09	-1.719E-07	-2.96E-09	-3.29E-09	-4.66E-07	-2.96E-09	-3.37E-09	-4.66E-07	2.20576E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	9.905E-07	-1.54E-08	-2.36E-08	-9.59E-09	-9.35E-08	-6.36E-08	-1.59E-08	-4.01E-06	-6.36E-08	-1.59E-08	9.90504E-07
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.08E+08	0.00E+00	0.00E+00	-4.29E+03	1.33E+00	0.00E+00	C_HgII_1_sed	1.606E-01	-2.41E-03	-3.83E-03	-1.29E-03	-9.59E-03	-1.07E-02	-1.91E-03	-9.59E-03	-1.09E-02	-1.92E-03	0.160566903
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	6.63E-01	-4.40E+03	0.00E+00	C_MeHg_1_sed	1.053E-04	-6.37E-07	-1.01E-06	-6.34E-05	-2.53E-06	-2.82E-06	-1.72E-04	-2.53E-06	-2.88E-06	-3.99E-04	0.000105314

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.004
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			0.050
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			0.101
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			0.229
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			0.808
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			0.229
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			0.050
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			0.014
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			0.624
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			0.036
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			9.90E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			5.01E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			9.99E-01
L_T,Hg0	Total Load, Hg0		g/yr	3.99E-01
L_T,HgII	Total Load, HgII		g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg		g/yr	7.43E-01
Rate Constants				
kw_v,Hg0	water column volatilization loss rate constant, Hg0		per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII		per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg		per yr	1.87
kw_oxid_1	water column oxidation rate constant		per yr	610.22
kw_oxid_2	water column oxidation rate constant		per yr	525.60
kw_red_1	water column reduction rate constant, layer 2		per yr	246.95
kw_red_2	water column reduction rate constant, layer 2		per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1		per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2		per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1		per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2		per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1		per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2		per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant		per yr	0.00
kb_oxid	benthic oxidation rate constant		per yr	0.00
kb_red	benthic reduction rate constant		per yr	0.00
kb_methy	benthic methylation rate constant		per yr	0.00
kb_demeth	benthic demethylation rate constant		per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant		per yr	0.00
v_sA	abiotic settling velocity		m/yr	4,792.63
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.030
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	1.65
TSS+2			mg/L	0.21
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1		L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 2		L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2		L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	1.80E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \quad \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.94E-05	19.36
C_HgII_1_Aq			g/m3	2.67E-06	2.67
C_MeHg_1_Aq			g/m3	9.97E-07	1.00
C_Hg0_2_Aq			g/m3	1.29E-04	128.72
C_HgII_2_Aq			g/m3	2.32E-04	231.58
C_MeHg_2_Aq			g/m3	5.61E-06	5.61
C_Hg0_pore			g/m3	1.29E-04	128.72
C_HgII_pore			g/m3	2.19E-04	218.65
C_MeHg_pore			g/m3	2.96E-06	2.96
C_HgT_1_filtered			g/m3	2.30E-05	23.03
C_HgT_2_filtered			g/m3	3.66E-04	365.90
C_HgT_Sed_filtered			g/m3	3.50E-04	350.33
C_Hg0_1_T			g/m3	1.94E-05	19.36
C_HgII_1_T			g/m3	7.24E-05	72.39
C_MeHg_1_T			g/m3	1.89E-06	1.89
C_Hg0_2_T			g/m3	1.29E-04	128.72
C_HgII_2_T			g/m3	7.11E-04	710.78
C_MeHg_2_T			g/m3	5.82E-06	5.82
C_Hg0_sed			g/m3	1.07E-04	106.83
C_HgII_1_sed			g/m3	1.83E+01	18330341.64
C_MeHg_1_sed			g/m3	4.90E-03	4901.52
C_Hg0_sed, wet			g/g	4.03E-11	0.000
C_HgII_1_sed, wet			g/g	1.43E-05	14.315
C_MeHg_1_sed, wet			g/g	5.87E-09	0.006
C_HgT_sed,wet			g/g	1.43E-05	14.321
C_Hg0_sed, dry weight			g/g	2.37E-10	0.00
C_HgII_1_sed, dry weight			g/g	4.07E-05	40.69
C_MeHg_1_sed, dry weight			g/g	1.09E-08	0.01
C_HgT_1			g/m3	9.36E-05	93.64
C_HgT_2			g/m3	8.45E-04	845.32
C_HgT_Sed			g/g	4.07E-05	40.70

			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		2.02%	77.31%	20.68%
Layer 2			0.69%	84.08%	15.23%
Sediments			0.03%	99.97%	0.00%

Q'	Bulk Exchange Flow		m3/yr	3,017,619
Qin	Inflow		m3/yr	3,474,314
Qout	Outflow		m3/yr	3,474,314
Aw	Surface Area of the Water Body		m2	378,381
E	Exchange rate		m2/yr	2
V_1	Volume of Layer 1	Aw*z_1	m3	183,741
V_2	Volume of Layer 2	Aw*z_2	m3	37,838
z1	depth of first water layer		m	0.49
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.63276%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.86115%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	5.59528%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.05171%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	43.95131%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	26.98508%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03204%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{Hg1,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red,1} \cdot V_w - kw_{methR} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{methR} \cdot V_w\right] \cdot C^w_{Hg2R} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s,A} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{Hg2R} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{methR} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{methR} \cdot V_w\right] \cdot C^w_{Hg2R} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{s,A} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{s,A} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{s,A} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T
C_HgII_1_T	1.12E+08	-6.02E+07	3.95E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	6.79E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.57E-01	C_MeHg_1_T
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	7.20E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	7.20E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	6.63E-01	-4.40E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix										x=b/A
1.936E-05	-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	1.94E-05	
7.239E-05	-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	7.24E-05	
1.888E-06	-2.70E-16	-5.31E-16	-1.54E-07	2.69E-15	-8.10E-16	-1.43E-07	3.74E-13	9.46E-08	-1.43E-07	1.89E-06	
1.287E-04	-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	0.000129	
7.108E-04	-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.000711	
5.824E-06	-4.780E-16	-1.048E-15	-1.715E-07	8.83E-15	-2.62E-15	-4.65E-07	1.22E-12	3.08E-07	-4.65E-07	5.82E-06	
1.068E-04	-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	0.000107	
1.833E+01	1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	18.33034	
4.902E-03	2.70E-14	-1.94E-13	-6.31E-05	8.91E-12	-7.60E-13	-1.71E-04	1.04E-09	2.64E-04	-3.98E-04	0.004902	

A*x=b

C T sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	1.65
TSS+2			mg/L	0.21
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_Hg0_1	Effective K for Hg0 in layer 2		L/kg	1.59E+07
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.43E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	1.80E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	7.51E-06	7.51
C_HgII_1_Aq			g/m3	1.04E-06	1.04
C_MeHg_1_Aq			g/m3	4.27E-07	0.43
C_Hg0_2_Aq			g/m3	4.87E-05	48.69
C_HgII_2_Aq			g/m3	8.76E-05	87.56
C_MeHg_2_Aq			g/m3	2.22E-06	2.22
C_Hg0_pore			g/m3	4.87E-05	48.69
C_HgII_pore			g/m3	8.26E-05	82.65
C_MeHg_pore			g/m3	1.14E-06	1.14
C_HgT_1_filtered			g/m3	8.97E-06	8.97
C_HgT_2_filtered			g/m3	1.38E-04	138.47
C_HgT_Sed_filtered			g/m3	1.32E-04	132.48
C_Hg0_1_T			g/m3	7.51E-06	7.51
C_HgII_1_T			g/m3	2.82E-05	28.15
C_MeHg_1_T			g/m3	8.09E-07	0.81
C_Hg0_2_T			g/m3	4.87E-05	48.69
C_HgII_2_T			g/m3	2.69E-04	268.75
C_MeHg_2_T			g/m3	2.31E-06	2.31
C_Hg0_sed			g/m3	4.04E-05	40.42
C_HgII_1_sed			g/m3	6.93E+00	6,928,453.97
C_MeHg_1_sed			g/m3	1.89E-03	1,891.81
C_Hg0_sed, wet			g/g	1.53E-11	0.00
C_HgII_1_sed, wet			g/g	5.41E-06	5.41
C_MeHg_1_sed, wet			g/g	2.27E-09	0.00
C_HgT_sed,wet			g/g	5.41E-06	5.41
C_Hg0_sed, dry weight			g/g	8.97E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.54E-05	15.38
C_MeHg_1_sed, dry weight			g/g	4.20E-09	0.00
C_HgT_1			g/m3	3.65E-05	36.47
C_HgT_2			g/m3	3.20E-04	319.75
C_HgT_Sed, dry weight			g/g	1.54E-05	15.38
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		2.22%	77.19%	20.59%
Layer 2			0.72%	84.05%	15.23%
Sediments			0.03%	99.97%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
z2	depth of second water layer		m	0	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.63276%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	8.86115%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	5.59528%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.05171%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	43.95131%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	26.98508%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	80.16218%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photoredW} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{biaHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHgII} A_w - v_{sB} \cdot f^{w,1}_{biaHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoredd} V_w - v_{sA} \cdot f^{w,1}_{abiMeHg} A_w - v_{sB} \cdot f^{w,1}_{biaMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photoredd} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abiHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{biaHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiHgII} A_w - v_{sB} \cdot f^{w,2}_{biaHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoredd} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiMeHg} A_w - v_{sB} \cdot f^{w,2}_{biaMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{sA} \cdot f^{w,2}_{abiaHg0} + v_{sB} \cdot f^{w,2}_{biaHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{sA} \cdot f^{w,2}_{abiaHgII} + v_{sB} \cdot f^{w,2}_{biaHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{sA} \cdot f^{w,2}_{abiaMeHg} + v_{sB} \cdot f^{w,2}_{biaMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed
	1	2	3	4	5	6	7	8	9
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_HgII_1_T	1.12E+08	-6.02E+07	3.95E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_MeHg_1_T	0.00E+00	6.79E-02	-9.84E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00
C_HgII_2_T	0.000E+00	1.134E+07	0.000E+00	1.99E+07	-1.15E+08	7.20E-01	0.00E+00	4.29E+03	0.00E+00
C_MeHg_2_T	0.000E+00	0.000E+00	3.626E+06	0.00E+00	7.20E-01	-4.88E+06	0.00E+00	0.00E+00	4.40E+03
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.62E+06	0.00E+00	6.63E-01	-4.40E+03

Target C_sed, wet 6.930386198 g/g

Matrix b	Solution Matrix	Inverted Matrix								x=b/A
C_Hg0_1_T	7.510E-06	-9.57E-09	-7.26E-09	-3.53E-09	-1.47E-09	-2.42E-10	-3.26E-09	-1.47E-09	1.04E-06	-3.02E-09	7.51E-06
C_HgII_1_T	2.815E-05	-1.79E-08	-3.03E-08	-6.51E-09	-3.15E-09	-9.04E-10	-5.82E-09	-3.13E-09	3.88E-06	-4.94E-09	2.82E-05
C_MeHg_1_T	8.093E-07	-2.70E-16	-5.31E-16	-1.54E-07	2.69E-15	-8.10E-16	-1.43E-07	3.74E-13	9.46E-08	-1.43E-07	8.09E-07
C_Hg0_2_T	4.869E-05	-1.624E-09	-1.533E-09	-2.047E-09	-4.53E-08	-1.64E-09	-4.48E-09	-4.53E-08	7.02E-06	-2.89E-09	4.87E-05
C_HgII_2_T	2.687E-04	-2.044E-09	-3.245E-09	1.352E-09	-8.12E-09	-9.05E-09	5.02E-09	-7.97E-09	3.88E-05	1.38E-08	0.000269
C_MeHg_2_T	2.308E-06	-4.780E-16	-1.048E-15	-1.715E-07	8.83E-15	-2.62E-15	-4.65E-07	1.22E-12	3.08E-07	-4.65E-07	2.31E-06
C_Hg0_sed	4.042E-05	-1.35E-09	-1.27E-09	-1.70E-09	-3.76E-08	-1.36E-09	-3.72E-09	-3.96E-06	5.82E-06	-2.40E-09	4.04E-05
C_HgII_1_sed	6.928E+00	1.35E-09	1.27E-09	6.31E-05	3.76E-08	1.36E-09	1.71E-04	3.96E-06	1.00E+00	3.98E-04	6.928454
C_MeHg_1_sed	1.892E-03	2.70E-14	-1.94E-13	-6.31E-05	8.91E-12	-7.60E-13	-1.71E-04	1.04E-09	2.64E-04	-3.98E-04	0.001892

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.38210%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.01183%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.01537%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		10.10022%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		80.80179%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		22.87564%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		5.03141%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		1.42443%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		62.40427%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.94994%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatiilization loss rate cc	per yr	388.36
kw_v,HgII	water column volatiilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatiilization loss rate cc	per yr	1.87
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	246.95
kw_red_2	water column reduction rate constant,	per yr	107.40
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for I	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for I	per yr	6.43
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	1.65
TSS+2		mg/L	0.21
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	1.59E+07
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.43E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	9.76E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	1.80E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} = \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS}$$
$$\frac{}{C_{diss,i}^j + C_{DOC,i}^j} \qquad \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w} \right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2} \right) Sc_{w,i}^{-0.67} \left(3.15 x 10^{7} \right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log\left(\mu_w\right) = \left[\frac{1301}{998.333 + 8.155\left(T_w - 20\right) + 0.00585\left(T_w - 20\right)^2} \right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.63276%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.59528%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			8.86115%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			16.16173%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05171%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			26.98508%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			43.95131%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			80.16218%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.38210%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.01537%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.01183%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03204%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			10.10222%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			80.80179%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			22.87564%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			5.03141%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			62.40427%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			1.42443%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			3.64405%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00099%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.05006%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99901%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.94994%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	1 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	0.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.06
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.09
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	548.69
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed}+K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6}+K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	127,696,640	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	31,924,160	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	127,696,640	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	1		TSS_1	1.65	mg/L
Sbio_zoo,1	0.5		TSS_2	0.21	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	6.23E-02				
Sbio_dead,2	8.73E-02				
S_abio, sed	5.28E+04				
S_bio_dead,sed	5.49E+02				
S_sed,total	5.34E+04	g/m3			

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			Solution	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b		Matrix							
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	2.01E+06	S_bio_dead,1	6.23E-02	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.062268
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	8.73E-02	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.08734
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	5.49E+02	0	0	0.000273	-2.50E-04	0	-3.07E-04	548.6925

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	1	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	0.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

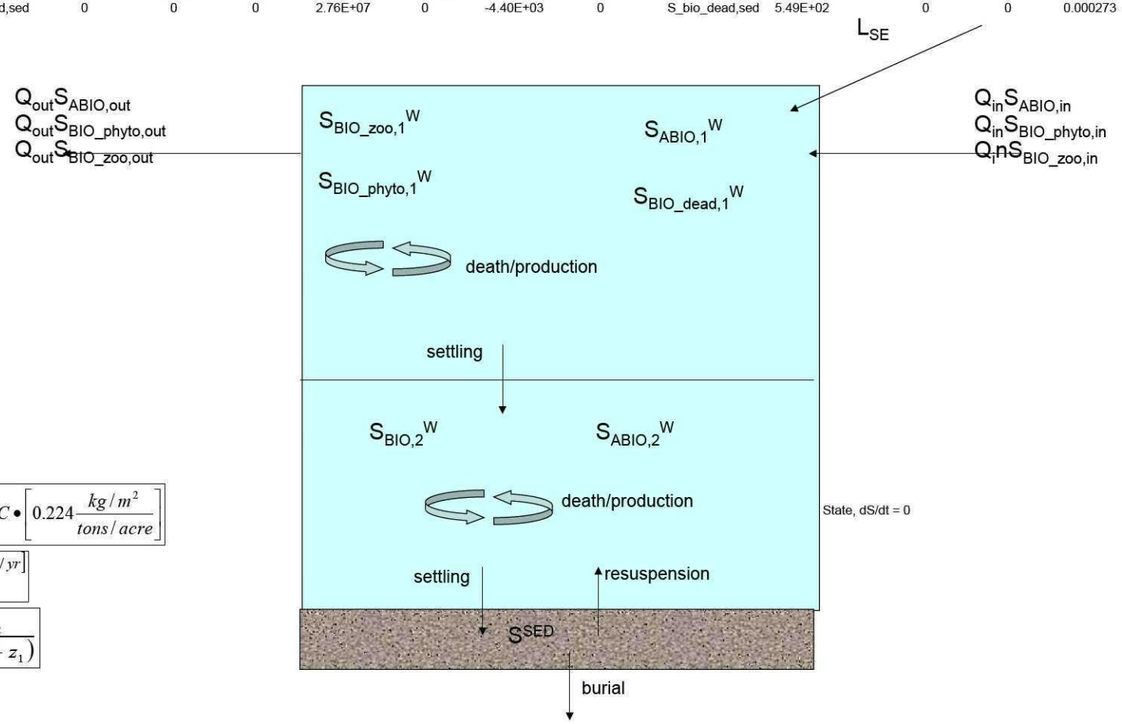
Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	0.00000016	1	2
k_meth_2	abiotic* methylation in layer 2		per day	0.0000016	1	4
k_meth_1	abiotic methylation in layer 1		per yr	0.0000584		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000584		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00633	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.05595		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03052		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.26985		
k_meth_1	abiotic methylation in layer 1		per yr	3.70E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.90E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC}\right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	0.00000016	1	2
k_meth_b	biotic methylation in sediments		per yr	0.0000584		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	0.000000016	1
k_demeth_2	biotic demethylation in layer 2		per day	0.00000016	
k_demeth_1	biotic demethylation in layer 1		per yr	0.00000584	
k_demeth_2	biotic demethylation in layer 2		per yr	0.0000584	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			6.33E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			5.60E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.05E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			2.70E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.15E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.90E-05	

$$k_{demeth} = k_{demeth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC}\right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608. mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	0.00000032	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.0001168		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Additional SERAFM Model Inputs and Outputs

Scenario 1 – Great Blue Heron

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations					
Hg0	0	g/m3			
HgII	5.64E-06	g/m3	5.64	-38.33653454	
MeHg	7.33E-08	g/m3	0.07332	43.0872112	Fish

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27	ug/g

Known Mercury in Contaminated Soils			
Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio		
HgII	7,182,936	1
MeHg	15,887	1

Kd_bio		
HgII	17,941,378	0.1405
MeHg	2,581,565	1

Kd_DOC		
HgII	301,427	1
MeHg	310,000	1

	PCT ERROR	CLEANUP
MeHg Filtered	9.50	15.95
HgT Filtered	-51.71	
MeHg Unfilter	-64.28	
HgT Unfiltere	-46.85	

Exposure Concentrations

		Scenario 1 With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2 Background Conditions		Scenario 3 Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	11.73	ng/L		-11.73	-100	0.47	ng/L	5.74	ng/L
	HgII Filtered	3.14	ng/L		-3.14	-100	0.13	ng/L	1.54	ng/L
Epilimnion	MeHg Filtered	0.43	ng/L	0.47525	0.04	9.5013533	0.03	ng/L	0.22	ng/L
	HgT Filtered	15.31	ng/L	7.39	-7.92	-51.71183	0.63	ng/L	7.50	ng/L
	Hg0 Unfiltered	11.73	ng/L		-11.73	-100	0.47	ng/L	5.74	ng/L
	HgII Unfiltered	66.10	ng/L		-66.10	-100	2.67	ng/L	32.34	ng/L
	MeHg Unfiltered	2.47	ng/L	0.88225	-1.59	-64.28243	0.18	ng/L	1.25	ng/L
	HgT Unfiltered	80.30	ng/L	42.67625	-37.62	-46.85323	3.32	ng/L	39.33	ng/L
Hypolimnion	Hg0 Filtered	21.98	ng/L		-21.98	-100	0.53	ng/L	10.57	ng/L
	HgII Filtered	116.08	ng/L		-116.08	-100	2.59	ng/L	55.68	ng/L
	MeHg Filtered	5.28	ng/L		-5.28	-100	0.23	ng/L	2.59	ng/L
	HgT Filtered	143.34	ng/L		-143.34	-100	3.36	ng/L	68.85	ng/L
	Hg0 Unfiltered	21.98	ng/L		-21.98	-100	0.53	ng/L	10.57	ng/L
	HgII Unfiltered	551.86	ng/L		-551.86	-100	12.34	ng/L	264.74	ng/L
	MeHg Unfiltered	7.89	ng/L		-7.89	-100	0.35	ng/L	3.87	ng/L
	HgT Unfiltered	581.74	ng/L		-581.74	-100	13.21	ng/L	279.19	ng/L
	Sediment									
	Hg0 porewater	21.98	ng/L		-21.98	-100	0.53	ng/L	10.568	ng/L
	HgII porewater	99.56	ng/L		-99.56	-100	2.18	ng/L	47.741	ng/L
	MeHg porewater	1.22	ng/L		-1.22	-100	0.05	ng/L	0.596	ng/L
	HgT porewater	122.77	ng/L		-122.77	-100	2.76	ng/L	58.905	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.22	ug/g		-33.22	-100	0.39	ug/g	15.93	ug/g
	MeHg bulk, dry	0.05107	ug/g	0.00422	-0.05	-91.73681	0.00	ug/g	0.02	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.730	ug/g	15.95	ug/g
	Trophic Level 3	0.40	ug/g		-0.40	-100	0.029	ug/g	0.20	ug/g
	Trophic Level 4	0.86	ug/g		-0.86	-100	0.063	ug/g	0.44	ug/g
	HI	1.97					0.14		1.00	
	Sensitive Indicator	Great Blue Heron					Great Blue Heron		Great Blue Heron	
	Target C_sed, dry	15.95	ug/g	Note: 8						
	Target C_sed, wet	7.19	ug/g							

Rate Constants

Process	Media	Value	Units		
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		ratio Sed
1.00E-03	Sediment	3.49E-07	per day		Meth/demeth
Demethylation	Epilimnion	1.16E-08	per day		50.00%
1.00E-03	Hypolimnion	1.16E-07	per day		
2.00E-03	Sediment	6.98E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

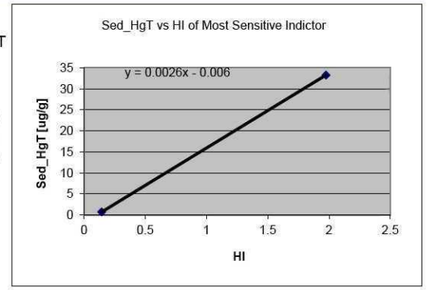
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.49	0.04	0.25
Otter	0.52	0.04	0.26
Mink	**1.02**	0.07	0.51
Great Blue Heron	**1.97**	0.14	**1.00**
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.93	0.07	0.47
Kingfisher	0.00	0.00	0.00
Wood Duck	0.36	0.03	0.18
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
1.97	33.27
0.14	0.73
m =	17.768
b=	-1.815
Sed_HgT	15.953
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.43	0.03	0.220	ng/L

Biota

Trophic Level 1: Phytoplankton	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Insects	0.07	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.40	0.03	0.20	ug Hg/ g wet weight
Trophic Level 4: Bass	0.86	0.06	0.44	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.47	0.03	0.24	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.04	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

Animal	Body Weight [kg in wet weight]	Ingestion Rate [kg wet weight/d]	Drinking rate [L/d]	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants --	Percent of Diet from Trophic Level 2 : Insects --	Percent of Diet from Trophic Level 2 : Crayfish or Frogs --	Percent of Diet from Trophic Level 3 : Fish --	Percent of Diet from Trophic Level 4 : Fish --	Percent of Diet from nonaquatic sources --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	36	0	0	0	36	75	0.49
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	29	9	39	75	0.52
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	70	76	75	**1.02**
Great Blue Heron	2.2	0.509	0.1	0%	5%	10%	50%	35%	0%	0	0	1	2	46	70	118	60	**1.97**
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	18	6	32	0	56	60	0.93
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	17	5	0	0	0	22	60	0.36
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	8	5000	0.00

Human

	Human Specific Parameters																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution 5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.005	0.00	2.64	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.08	2.14	0.62	3	75	0.04
0.003	0.00	0.00	0.27	0.19	5.06	6	75	0.07
0.001	0.00	0.06	0.13	3.33	5.07	9	60	0.14
0.015	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.002	0.00	1.27	0.46	2.32	0.00	4	60	0.07
0.004	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.002	1.22	0.36	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.03	0.08	0.48	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.035	0.00	18.45	0.00	0.00	0.00	18	75	0.25
0.018	0.00	0.00	0.59	14.92	4.33	20	75	0.26
0.022	0.00	0.00	1.87	1.35	35.35	39	75	0.51
0.010	0.00	0.42	0.92	23.24	35.42	60	60	**1.00**
0.103	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.016	0.00	8.87	3.19	16.19	0.00	28	60	0.47
0.025	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.015	8.49	2.50	0.00	0.00	0.00	11	60	0.18
0.000	0.00	0.00	0.22	0.55	3.35	4	5000	0.00
							RfD	
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Great Blue Heron

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Great Blue Heron

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893.2	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.71E-07	0.47
C_HgII_1_Aq			g/m3	1.27E-07	0.13
C_MeHg_1_Aq			g/m3	3.15E-08	0.03
C_Hg0_2_Aq			g/m3	5.32E-07	0.53
C_HgII_2_Aq			g/m3	2.59E-06	2.59
C_MeHg_2_Aq			g/m3	2.31E-07	0.23
C_Hg0_pore			g/m3	5.32E-07	0.53
C_HgII_pore			g/m3	2.18E-06	2.18
C_MeHg_pore			g/m3	4.76E-08	0.05
C_HgT_1_filtered			g/m3	6.30E-07	0.63
C_HgT_2_filtered			g/m3	3.36E-06	3.36
C_HgT_Sed_filtered			g/m3	2.76E-06	2.76
C_Hg0_1_T			g/m3	4.71E-07	0.47
C_HgII_1_T			g/m3	2.67E-06	2.67
C_MeHg_1_T			g/m3	1.79E-07	0.18
C_Hg0_2_T			g/m3	5.32E-07	0.53
C_HgII_2_T			g/m3	1.23E-05	12.34
C_MeHg_2_T			g/m3	3.45E-07	0.35
C_Hg0_sed_bulk			g/m3	4.42E-07	0
C_HgII_1_sed_bulk			g/m3	3.28E-01	328,097
C_MeHg_1_sed_bulk			g/m3	8.97E-04	897
C_Hg0_sed_wet			g/g	3.45E-13	0.000
C_HgII_1_sed_wet			g/g	3.93E-07	0.393
C_MeHg_1_sed_wet			g/g	6.65E-14	0.000
C_HgT_sed,wet			g/g	3.93E-07	0.393
C_Hg0_sed_dry weight			g/g	9.80E-13	0.0000
C_HgII_1_sed_dry weight			g/g	7.28E-07	0.7283
C_MeHg_1_sed_dry weight			g/g	1.99E-09	0.0020
C_HgT_1			g/m3	3.32E-06	3.321
C_HgT_2			g/m3	1.32E-05	13.213
C_HgT_Sed_dry weight			g/g	7.30E-07	0.730

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg T/Hg T)	5.40%	80.41%	14.19%
Layer 2		2.61%	93.36%	4.03%
Sediments		0.27%	99.73%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V_1	Volume of Layer 1	Aw*z_1	m3	648,711
V_2	Volume of Layer 2	Aw*z_2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			1.000
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			0.029
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.036
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			0.112
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.039
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			0.146
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.174
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			0.557

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photoreW} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{z1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{zB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{z1} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{zB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoredW} V_w - v_{z1} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{zB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photoredW} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{z1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{zB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{z1} \cdot f^{w,2}_{abioHgII} A_w - v_{zB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{z1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{zB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{z1} \cdot f^{w,2}_{abioHg0} + v_{zB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{z1} \cdot f^{w,2}_{abioHgII} + v_{zB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{z1} \cdot f^{w,2}_{abioMeHg} + v_{zB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed
	1	2	3	4	5	6	7	8	9
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E+08	0.00E+00	0.00E+00	-5.25E+03	3.54E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00

Matrix b	Solution Matrix
C_Hg0_1_T	4.712E-07
C_HgII_1_T	2.670E-06
C_MeHg_1_T	1.792E-07
C_Hg0_2_T	5.321E-07
C_HgII_2_T	1.234E-05
C_MeHg_2_T	3.452E-07
C_Hg0_sed	4.417E-07
C_HgII_1_sed	3.281E-01
C_MeHg_1_sed	8.968E-04

Inverted Matrix

C_Hg0_1_T	-8.13E-09	-7.48E-09	-3.10E-09	-7.60E-09	-7.47E-09	-3.13E-09	-7.60E-09	-7.47E-09	-3.14E-09
C_HgII_1_T	-3.39E-08	-4.26E-08	-1.30E-08	-4.05E-08	-4.21E-08	-1.32E-08	-4.05E-08	-4.21E-08	-1.32E-08
C_MeHg_1_T	-6.58E-10	-8.19E-10	-8.94E-08	-1.33E-09	-1.49E-09	-8.87E-08	-1.33E-09	-1.52E-09	-8.86E-08
C_Hg0_2_T	-7.220E-09	-8.479E-09	-2.945E-09	-4.60E-08	-1.42E-08	-3.24E-09	-4.60E-08	-1.42E-08	-3.25E-09
C_HgII_2_T	-1.581E-07	-1.968E-07	-6.130E-08	-3.19E-07	-3.58E-07	-6.34E-08	-3.19E-07	-3.58E-07	-6.36E-08
C_MeHg_2_T	-2.166E-09	-2.697E-09	-1.236E-07	-4.38E-09	-4.91E-09	-2.92E-07	-4.38E-09	-5.00E-09	-2.92E-07
C_Hg0_sed	-5.99E-09	-7.04E-09	-2.44E-09	-3.82E-08	-1.18E-08	-2.69E-09	-3.24E-06	-1.18E-08	-2.69E-09
C_HgII_1_sed	-4.20E-03	-5.23E-03	-1.63E-03	-8.49E-03	-9.52E-03	-1.69E-03	-8.49E-03	-9.71E-03	-1.69E-03
C_MeHg_1_sed	-6.35E-06	-7.91E-06	-2.82E-04	-1.28E-05	-1.44E-05	-6.66E-04	-1.28E-05	-1.47E-05	-8.55E-04

x=b/A
4.71217E-07
2.67016E-06
1.79194E-07
5.3214E-07
1.23359E-05
3.45194E-07
4.41677E-07
0.328097233
0.000896776

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.008
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.052
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.091
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.732
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.121
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.063
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.738
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.330
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		5.52E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		4.40E-05
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2]\left[H^+\right]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \cdot \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS} = \frac{C_{unfiltered,i}^{j}}{C_{diss,i}^{j}+C_{DOC,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.17E-05	11.73
C_HgII_1_Aq			g/m3	3.14E-06	3.14
C_MeHg_1_Aq			g/m3	4.34E-07	0.43
C_Hg0_2_Aq			g/m3	2.20E-05	21.98
C_HgII_2_Aq			g/m3	1.16E-04	116.08
C_MeHg_2_Aq			g/m3	5.28E-06	5.28
C_Hg0_pore			g/m3	2.20E-05	21.98
C_HgII_pore			g/m3	9.96E-05	99.56
C_MeHg_pore			g/m3	1.22E-06	1.22
C_HgT_1_filtered			g/m3	1.53E-05	15.31
C_HgT_2_filtered			g/m3	1.43E-04	143.34
C_HgT_Sed_filtered			g/m3	1.23E-04	122.77
C_Hg0_1_T			g/m3	1.17E-05	11.73
C_HgII_1_T			g/m3	6.61E-05	66.10
C_MeHg_1_T			g/m3	2.47E-06	2.47
C_Hg0_2_T			g/m3	2.20E-05	21.98
C_HgII_2_T			g/m3	5.52E-04	551.86
C_MeHg_2_T			g/m3	7.89E-06	7.89
C_Hg0_sed			g/m3	1.82E-05	18.25
C_HgII_1_sed			g/m3	1.50E+01	14965109.78
C_MeHg_1_sed			g/m3	2.30E-02	23006.97
C_Hg0_sed, wet			g/g	6.89E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.687
C_MeHg_1_sed, wet			g/g	2.75E-08	0.028
C_HgT_sed,wet			g/g	1.17E-05	11.714
C_Hg0_sed, dry weight			g/g	4.05E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.32E-05	33.22
C_MeHg_1_sed, dry weight			g/g	5.11E-08	0.05
C_HgT_1			g/m3	8.03E-05	80.30
C_HgT_2			g/m3	5.82E-04	581.74
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.08%	82.31%	14.61%
Layer 2			1.36%	94.86%	3.78%
Sediments			0.15%	99.85%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.81571%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	2.94813%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	3.61221%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.93402%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	14.62272%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	17.42109%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03550%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red,1} \cdot V_w - kw_{metR} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg1}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{metB} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demetR} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg1} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg1} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg1} + \left[-Q' - kw_{red2} \cdot V_w - kw_{metR} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII}\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{metB2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demetR} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2} + Q' \cdot C^w_{MeHg1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2) from Mortimer, cited in Schnoor, 1996, pg. 57. for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix											x=b/A
1.173E-05	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	1.17E-05	C_Hg0_1_T	
6.610E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	6.61E-05	C_HgII_1_T	
2.470E-06	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	2.47E-06	C_MeHg_1_T	
2.198E-05	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	2.2E-05	C_Hg0_2_T	
5.519E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.000552	C_HgII_2_T	
7.888E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	7.89E-06	C_MeHg_2_T	
1.825E-05	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	1.82E-05	C_Hg0_sed	
1.497E+01	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	14.96511	C_HgII_1_sed	
2.301E-02	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.023007	C_MeHg_1_sed	

A*x=b

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

C_T_sed 14.988135 g/m3

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	13900.95
TSS_1			mg/L	8.46
TSS+2			mg/L	1.34
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_Hg0_1	Effective K for Hg0 in layer 2		L/kg	2.37E+06
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.54E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	3.69E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	5.74E-06	5.74
C_HgII_1_Aq			g/m3	1.54E-06	1.54
C_MeHg_1_Aq			g/m3	2.20E-07	0.22
C_Hg0_2_Aq			g/m3	1.06E-05	10.57
C_HgII_2_Aq			g/m3	5.57E-05	55.68
C_MeHg_2_Aq			g/m3	2.59E-06	2.59
C_Hg0_pore			g/m3	1.06E-05	10.57
C_HgII_pore			g/m3	4.77E-05	47.74
C_MeHg_pore			g/m3	5.96E-07	0.60
C_HgT_1_filtered			g/m3	7.50E-06	7.50
C_HgT_2_filtered			g/m3	6.88E-05	68.85
C_HgT_Sed_filtered			g/m3	5.89E-05	58.91
C_Hg0_1_T			g/m3	5.74E-06	5.74
C_HgII_1_T			g/m3	3.23E-05	32.34
C_MeHg_1_T			g/m3	1.25E-06	1.25
C_Hg0_2_T			g/m3	1.06E-05	10.57
C_HgII_2_T			g/m3	2.65E-04	264.74
C_MeHg_2_T			g/m3	3.87E-06	3.87
C_Hg0_sed			g/m3	8.77E-06	8.77
C_HgII_1_sed			g/m3	7.18E+00	7,175,755.69
C_MeHg_1_sed			g/m3	1.12E-02	11,240.63
C_Hg0_sed, wet			g/g	3.31E-12	0.00
C_HgII_1_sed, wet			g/g	5.60E-06	5.60
C_MeHg_1_sed, wet			g/g	1.35E-08	0.01
C_HgT_sed,wet			g/g	5.62E-06	5.62
C_Hg0_sed, dry weight			g/g	1.95E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.59E-05	15.93
C_MeHg_1_sed, dry weight			g/g	2.50E-08	0.02
C_HgT_1			g/m3	3.93E-05	39.33
C_HgT_2			g/m3	2.79E-04	279.19
C_HgT_Sed, dry weight			g/g	1.60E-05	15.95
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.18%	82.23%	14.59%
Layer 2			1.39%	94.83%	3.79%
Sediments			0.16%	99.84%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{biaHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{biaHgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abiMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{biaMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abiHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{biaHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiHgII} A_w - v_{sB} \cdot f^{w,2}_{biaHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiaMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{biaMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abiaHg0} + v_{sB} \cdot f^{w,2}_{biaHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abiaHgII} + v_{sB} \cdot f^{w,2}_{biaHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abiaMeHg} + v_{sB} \cdot f^{w,2}_{biaMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed	Matrix b		Solution Matrix	Inverted Matrix								x=b/A
	1	2	3	4	5	6	7	8	9	b		Matrix									
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	5.740E-06	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	5.74E-06
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	3.234E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	3.23E-05
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T	1.251E-06	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	1.25E-06
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.057E-05	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	1.06E-05
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	2.647E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.000265
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T	3.874E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	3.87E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	8.771E-06	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	8.77E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	7.19E+00	C_HgII_1_sed	7.176E+00	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	7.175756
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	-5.26E+03	C_MeHg_1_sed	1.124E-02	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.011241

A*x=b

Target C_sed, wet 7.18700509 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatiilization loss rate cc	per yr	134.70
kw_v,HgII	water column volatiilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatiilization loss rate cc	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	122.63
kw_red_2	water column reduction rate constant,	per yr	23.27
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for l	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for l	per yr	0.82
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.153 \text{x} 10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \Big/ \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{TSS}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.81571%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61221%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			2.94813%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93402%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			17.42109%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			14.62272%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.78562%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.16164%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00628%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.14683%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			73.17463%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.14319%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			73.80506%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			6.31498%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.99560%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.83
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	1.14
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	7,154.39
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed}+K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6}+K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,344	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	8.46	mg/L
Sbio_zoo,1	2.5		TSS_2	1.34	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	8.30E-01				
Sbio_dead,2	1.14E+00				
S_abio, sed	8.42E+04				
S_bio_dead,sed	7.15E+03				
S_sed,total	9.14E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

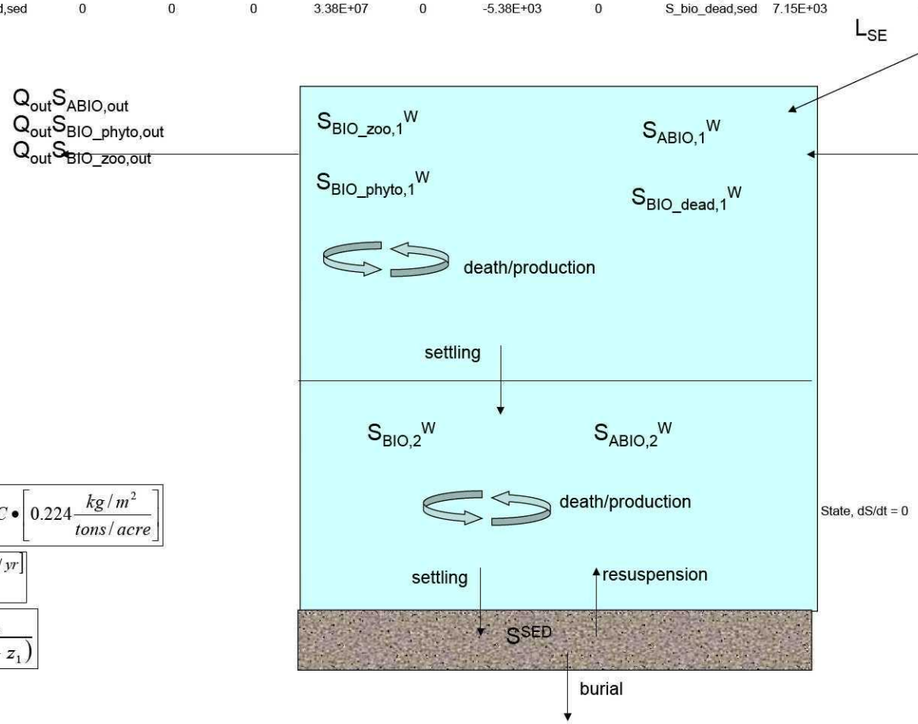
Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$
$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed			Solution	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b		Matrix							
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	3.55E+07	S_bio_dead,1	8.30E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.829741
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	1.14E+00	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	1.138825
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	7.15E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	7154.393



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

1 Modeled from Wetzel.	Oligo	Meso	Eutro	Dystro
Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
Used (mg C/m3)	60	200	500	125
Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankton (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

5 Modeled from Wetzel				
Wetzel (mg C/m2/day)	50-300	250-1000	>1000	<50-500
Used (mg C/m2/day)	175	625	1250	275
Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abiq2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00816	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.03612		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03934		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.17421		
k_meth_1	abiotic methylation in layer 1		per yr	3.46E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	8.93E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.16E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.74E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.02E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	8.93E-06	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1	
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02		
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03		
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00		
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01		

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	1
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

$$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$$

1 UV-B is modeled as being 0.5% of visible light.
check?

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Pied-Billed Grebe

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Kd_abio		
HgII	7,182,936	1
MeHg	15,887	1
Kd_bio		
HgII	17,941,378	1
MeHg	2,581,565	1
Kd_DOC		
HgII	301,427	1
MeHg	310,000	1
	PCT ERROR	CLEANUP
MeHg Filtered	9.50	35.93
HgT Filtered	-51.71	
MeHg Unfilte	-64.28	
HgT Unfiltere	-46.85	

Inflow Mercury Concentrations

Hg0	0	g/m3	5.64	-38.33653462	
HgII	5.64E-06	g/m3	0.07332	43.08721129	Fish
MeHg	7.33E-08	g/m3			

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27	ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	11.73	ng/L		-11.73	-100	0.47	ng/L	12.65	ng/L
	HgII Filtered	3.14	ng/L		-3.14	-100	0.13	ng/L	3.39	ng/L
Epilimnion	MeHg Filtered	0.43	ng/L	0.47525	0.04	9.5013533	0.03	ng/L	0.47	ng/L
	HgT Filtered	15.31	ng/L	7.39	-7.92	-51.71183	0.63	ng/L	16.50	ng/L
	Hg0 Unfiltered	11.73	ng/L		-11.73	-100	0.47	ng/L	12.65	ng/L
	HgII Unfiltered	66.10	ng/L		-66.10	-100	2.67	ng/L	71.27	ng/L
	MeHg Unfiltered	2.47	ng/L	0.88225	-1.59	-64.28243	0.18	ng/L	2.66	ng/L
	HgT Unfiltered	80.30	ng/L	42.67625	-37.62	-46.85323	3.32	ng/L	86.58	ng/L
Hypolimnion	Hg0 Filtered	21.98	ng/L		-21.98	-100	0.53	ng/L	23.73	ng/L
	HgII Filtered	116.08	ng/L		-116.08	-100	2.59	ng/L	125.34	ng/L
	MeHg Filtered	5.28	ng/L		-5.28	-100	0.23	ng/L	5.69	ng/L
	HgT Filtered	143.34	ng/L		-143.34	-100	3.36	ng/L	154.76	ng/L
	Hg0 Unfiltered	21.98	ng/L		-21.98	-100	0.53	ng/L	23.73	ng/L
	HgII Unfiltered	551.86	ng/L		-551.86	-100	12.34	ng/L	595.89	ng/L
	MeHg Unfiltered	7.89	ng/L		-7.89	-100	0.35	ng/L	8.50	ng/L
	HgT Unfiltered	581.74	ng/L		-581.74	-100	13.21	ng/L	628.13	ng/L
	Sediment									
	Hg0 porewater	21.98	ng/L		-21.98	-100	0.53	ng/L	23.734	ng/L
	HgII porewater	99.56	ng/L		-99.56	-100	2.18	ng/L	107.511	ng/L
	MeHg porewater	1.22	ng/L		-1.22	-100	0.05	ng/L	1.316	ng/L
	HgT porewater	122.77	ng/L		-122.77	-100	2.76	ng/L	132.561	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.22	ug/g		-33.22	-100	0.39	ug/g	35.87	ug/g
	MeHg bulk, dry	0.05107	ug/g	0.00422	-0.05	-91.73681	0.00	ug/g	0.06	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.730	ug/g	35.93	ug/g
	Trophic Level 3	0.40	ug/g		-0.40	-100	0.029	ug/g	0.43	ug/g
	Trophic Level 4	0.86	ug/g		-0.86	-100	0.063	ug/g	0.93	ug/g
	HI	0.93					0.07		1.00	
	Sensitive Indicator	Pied-bill Grebe					Pied-bill Grebe		Pied-bill Grebe	
	Target C_sed, dry	35.93	ug/g	Note: 8						
	Target C_sed, wet	16.18	ug/g							

Rate Constants

Process	Media	Value	Units		
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		ratio Sed
1.00E-03	Sediment	3.49E-07	per day		Meth/demeth
Demethylation	Epilimnion	1.16E-08	per day		50.00%
1.00E-03	Hypolimnion	1.16E-07	per day		
2.00E-03	Sediment	6.98E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

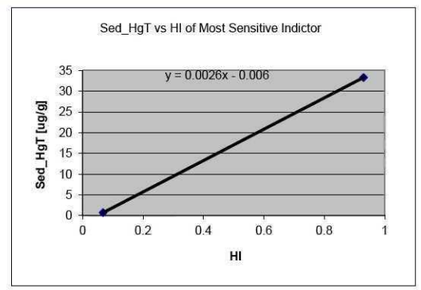
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.49	0.04	0.52
Otter	0.52	0.04	0.56
Mink	0.00	0.00	0.00
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.93	0.07	**1.00**
Kingfisher	0.00	0.00	0.00
Wood Duck	0.36	0.03	0.39
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
0.93	33.27
0.07	0.73
m =	37.740
b=	-1.815
Sed_HgT	35.925
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.

Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

	Site-Specific User Input	Required
	Model Calculated	No input required
	Data Necessary for certain sites	Only necessary if applicable to site of interest
	Scenario 1 Output	
	Scenario 2 Output	
	Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.43	0.03	0.467	ng/L

Biota

Trophic Level 1: Phytoplankton	0.08	0.01	0.09	ug Hg/ g wet weight
Trophic Level 2: Insects	0.07	0.01	0.08	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.08	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.40	0.03	0.43	ug Hg/ g wet weight
Trophic Level 4: Bass	0.86	0.06	0.93	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.47	0.03	0.50	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.08	0.01	0.09	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.08	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

Animal	Body Weight [kg in wet weight]	Ingestion Rate [kg wet weight/d]	Drinking rate [L/d]	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants --	Percent of Diet from Trophic Level 2 : Insects --	Percent of Diet from Trophic Level 2 : Crayfish or Frogs --	Percent of Diet from Trophic Level 3 : Fish --	Percent of Diet from Trophic Level 4 : Fish --	Percent of Diet from nonaquatic sources --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	36	0	0	0	36	75	0.49
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	29	9	39	75	0.52
Mink	0.85	0.1145	0.085	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	75	0.00
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	18	6	32	0	56	60	0.93
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	17	5	0	0	0	22	60	0.36
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	8	5000	0.00
Human																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution 5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.005	0.00	2.64	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.08	2.14	0.62	3	75	0.04
0.003	0.00	0.00	0.00	0.00	0.00	0	75	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.015	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.002	0.00	1.27	0.46	2.32	0.00	4	60	0.07
0.004	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.002	1.22	0.36	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.03	0.08	0.48	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.075	0.00	39.19	0.00	0.00	0.00	39	75	0.52
0.039	0.00	0.00	1.25	31.70	9.20	42	75	0.56
0.047	0.00	0.00	0.00	0.00	0.00	0	75	0.00
0.021	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.220	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.034	0.00	18.85	6.77	34.38	0.00	60	60	**1.00**
0.053	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.031	18.03	5.31	0.00	0.00	0.00	23	60	0.39
0.000	0.00	0.00	0.47	1.16	7.12	9	5000	0.00
							RfD	
0.008	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Pied-Billed Grebe

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Pied-Billed Grebe

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Coun	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeHg	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Pied-Billed Grebe

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and reflec		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

this table does not all correspond to EPA Report to Congress - check!

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	
HgII	Mean	58,000	50000	100,000	200,000	
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000		
MeHg	Mean	7000	3000	100,000	500,000	
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000		
Hg0		1,000	1,000	3000	1,000	NTG added these 11/1/19

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893.2	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.71E-07	0.47
C_HgII_1_Aq			g/m3	1.27E-07	0.13
C_MeHg_1_Aq			g/m3	3.15E-08	0.03
C_Hg0_2_Aq			g/m3	5.32E-07	0.53
C_HgII_2_Aq			g/m3	2.59E-06	2.59
C_MeHg_2_Aq			g/m3	2.31E-07	0.23
C_Hg0_pore			g/m3	5.32E-07	0.53
C_HgII_pore			g/m3	2.18E-06	2.18
C_MeHg_pore			g/m3	4.76E-08	0.05
C_HgT_1_filtered			g/m3	6.30E-07	0.63
C_HgT_2_filtered			g/m3	3.36E-06	3.36
C_HgT_Sed_filtered			g/m3	2.76E-06	2.76
C_Hg0_1_T			g/m3	4.71E-07	0.47
C_HgII_1_T			g/m3	2.67E-06	2.67
C_MeHg_1_T			g/m3	1.79E-07	0.18
C_Hg0_2_T			g/m3	5.32E-07	0.53
C_HgII_2_T			g/m3	1.23E-05	12.34
C_MeHg_2_T			g/m3	3.45E-07	0.35
C_Hg0_sed, bulk			g/m3	4.42E-07	0
C_HgII_1_sed, bulk			g/m3	3.28E-01	328,097
C_MeHg_1_sed, bulk			g/m3	8.97E-04	897
C_Hg0_sed, wet			g/g	3.45E-13	0.000
C_HgII_1_sed, wet			g/g	3.93E-07	0.393
C_MeHg_1_sed, wet			g/g	6.65E-14	0.000
C_HgT_sed,wet			g/g	3.93E-07	0.393
C_Hg0_sed, dry weight			g/g	9.80E-13	0.0000
C_HgII_1_sed, dry weight			g/g	7.28E-07	0.7283
C_MeHg_1_sed, dry weight			g/g	1.99E-09	0.0020
C_HgT_1			g/m3	3.32E-06	3.321
C_HgT_2			g/m3	1.32E-05	13.213
C_HgT_Sed, dry weight			g/g	7.30E-07	0.730
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		5.40%	80.41%	14.19%
Layer 2			2.61%	93.36%	4.03%
Sediments			0.27%	99.73%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			1.000	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.008	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			0.029	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			1.000	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.036	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			0.112	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.000	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.039	
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			0.146	
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.000	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.174	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			0.557	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{vol Hg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{1A} \cdot f^{w,1}_{abio Hg0} \cdot A_w - v_{1B} \cdot f^{w,1}_{bio Hg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{vol HgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{1A} \cdot f^{w,1}_{abio HgII} A_w - v_{1B} \cdot f^{w,1}_{bio HgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{vol MeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{1A} \cdot f^{w,1}_{abio MeHg} \cdot A_w - v_{1B} \cdot f^{w,1}_{bio MeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{2A} \cdot f^{w,2}_{abio Hg0} \cdot A_w - v_{2B} \cdot f^{w,2}_{bio Hg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq Hg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aq Hg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sed Hg0}\right] \cdot A_w \cdot C^{sed}_{aq Hg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{2A} \cdot f^{w,2}_{abio HgII} A_w - v_{2B} \cdot f^{w,2}_{bio HgII} A_w - R_{sw} \cdot f^{w,2}_{aq HgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aq HgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sed HgII} A_w\right] \cdot C^{sed}_{aq HgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth,2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{2A} \cdot f^{w,2}_{abio MeHg} \cdot A_w - v_{2B} \cdot f^{w,2}_{bio MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aq Hg0} + \left(v_{2A} \cdot f^{w,2}_{abio Hg0} + v_{2B} \cdot f^{w,2}_{bio Hg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aq Hg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,Hg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aq HgII} + \left(v_{2A} \cdot f^{w,2}_{abio HgII} + v_{2B} \cdot f^{w,2}_{bio HgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aq HgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed HgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aq MeHg} + \left(v_{2A} \cdot f^{w,2}_{abio MeHg} + v_{2B} \cdot f^{w,2}_{bio MeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aq MeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,MeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C Hg0 1 T	C HgII 1 T	C MeHg 1 T	C Hg0 2 T	C HgII 2 T	C MeHg 2 T	C Hg0 1 sed	C HgII 1 sed	C MeHg 1 sed
	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	5.25E+03	0.00E+00	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E+08	0.00E+00	0.00E+00	-5.25E+03	3.54E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03

A*x=b

Matrix b		Solution Matrix
-4.89E-01	C Hg0 1 T	4.712E-07
-6.18E+01	C HgII 1 T	2.670E-06
-1.43E+00	C MeHg 1 T	1.792E-07
0.00E+00	C Hg0 2 T	5.321E-07
0.00E+00	C HgII 2 T	1.234E-05
0.00E+00	C MeHg 2 T	3.452E-07
0.00E+00	C Hg0 sed	4.417E-07
0.00E+00	C HgII 1 sed	3.281E-01
0.00E+00	C MeHg 1 sed	8.968E-04

Inverted Matrix

-8.13E-09	-7.48E-09	-3.10E-09	-7.60E-09	-7.47E-09	-3.13E-09	-7.60E-09	-7.47E-09	-3.14E-09	4.71217E-07
-3.39E-08	-4.26E-08	-1.30E-08	-4.05E-08	-4.21E-08	-1.32E-08	-4.05E-08	-4.21E-08	-1.32E-08	2.67016E-06
-6.58E-10	-8.19E-10	-8.94E-08	-1.33E-09	-1.49E-09	-8.87E-08	-1.33E-09	-1.52E-09	-8.86E-08	1.79194E-07
-7.220E-09	-8.479E-09	-2.945E-09	-4.60E-08	-1.42E-08	-3.24E-09	-4.60E-08	-1.42E-08	-3.25E-09	5.3214E-07
-1.581E-07	-1.968E-07	-6.130E-08	-3.19E-07	-3.58E-07	-6.34E-08	-3.19E-07	-3.58E-07	-6.36E-08	1.23359E-05
-2.166E-09	-2.697E-09	-1.236E-07	-4.38E-09	-4.91E-09	-2.92E-07	-4.38E-09	-5.00E-09	-2.92E-07	3.45194E-07
-5.99E-09	-7.04E-09	-2.44E-09	-3.82E-08	-1.18E-08	-2.69E-09	-3.24E-06	-1.18E-08	-2.69E-09	4.41677E-07
-4.20E-03	-5.23E-03	-1.63E-03	-8.49E-03	-9.52E-03	-1.69E-03	-8.49E-03	-9.71E-03	-1.69E-03	0.328097232
-6.35E-06	-7.91E-06	-2.82E-04	-1.28E-05	-1.44E-05	-6.66E-04	-1.28E-05	-1.47E-05	-8.55E-04	0.000896776

x=b/A

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.008
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.052
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.091
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.732
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.121
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.063
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.738
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.330
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		5.52E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		4.40E-05
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}}}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.17E-05	11.73
C_HgII_1_Aq			g/m3	3.14E-06	3.14
C_MeHg_1_Aq			g/m3	4.34E-07	0.43
C_Hg0_2_Aq			g/m3	2.20E-05	21.98
C_HgII_2_Aq			g/m3	1.16E-04	116.08
C_MeHg_2_Aq			g/m3	5.28E-06	5.28
C_Hg0_pore			g/m3	2.20E-05	21.98
C_HgII_pore			g/m3	9.96E-05	99.56
C_MeHg_pore			g/m3	1.22E-06	1.22
C_HgT_1_filtered			g/m3	1.53E-05	15.31
C_HgT_2_filtered			g/m3	1.43E-04	143.34
C_HgT_Sed_filtered			g/m3	1.23E-04	122.77
C_Hg0_1_T			g/m3	1.17E-05	11.73
C_HgII_1_T			g/m3	6.61E-05	66.10
C_MeHg_1_T			g/m3	2.47E-06	2.47
C_Hg0_2_T			g/m3	2.20E-05	21.98
C_HgII_2_T			g/m3	5.52E-04	551.86
C_MeHg_2_T			g/m3	7.89E-06	7.89
C_Hg0_sed			g/m3	1.82E-05	18.25
C_HgII_1_sed			g/m3	1.50E+01	14965109.78
C_MeHg_1_sed			g/m3	2.30E-02	23006.97
C_Hg0_sed, wet			g/g	6.89E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.687
C_MeHg_1_sed, wet			g/g	2.75E-08	0.028
C_HgT_sed,wet			g/g	1.17E-05	11.714
C_Hg0_sed, dry weight			g/g	4.05E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.32E-05	33.22
C_MeHg_1_sed, dry weight			g/g	5.11E-08	0.05
C_HgT_1			g/m3	8.03E-05	80.30
C_HgT_2			g/m3	5.82E-04	581.74
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.08%	82.31%	14.61%
Layer 2			1.36%	94.86%	3.78%
Sediments			0.15%	99.85%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.81571%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	2.94813%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	3.61221%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.93402%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	14.62272%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	17.42109%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03550%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot A_w \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix									x=b/A
1.173E-05	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	1.17E-05
6.610E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	6.61E-05
2.470E-06	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	2.47E-06
2.198E-05	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	2.2E-05
5.519E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.000552
7.888E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	7.89E-06
1.825E-05	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	1.82E-05
1.497E+01	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	14.96511
2.301E-02	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.023007

C_T_sed 14.988135 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1 - \theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	orgaanic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	orgaanic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	orgaanic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	orgaanic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \times 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity		m/yr		4792.628412
v_sB	biotic settling velocity		m/yr		73
v_rs	resuspension velocity		m/yr		0.003700005
k_mort	phytoplankton mortality rate		per yr		10.95
v_min	mineralization rate		per yr		0.01
v_bur	burial rate		m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0			m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII			m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg			m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0			m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII			m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg			m2/sec	6.11E-10
rho_s	Sediment Particle Density			g/cm3	2.65E+00
θ_sed	sediment porosity			cm3/cm3	0.83
z_sed	sediment layer,char mixing length			m	0.03
V_sed	Volume of Sediment	Aw*z_sed		m3	13900.95
TSS_1				mg/L	8.46
TSS+2				mg/L	1.34
Effective Partition Coefficients for each Hg species and layer					
K_eff_Hg0_1	Effective K for Hg0 in layer 1			L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2			L/kg	2.37E+06
K_eff_MeHg_1	Effective K for HgII in layer 1			L/kg	5.54E+05
K_eff_Hg0_2	Effective K for HgII in layer 2			L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1			L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2			L/kg	3.69E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.27E-05	12.65
C_HgII_1_Aq			g/m3	3.39E-06	3.39
C_MeHg_1_Aq			g/m3	4.67E-07	0.47
C_Hg0_2_Aq			g/m3	2.37E-05	23.73
C_HgII_2_Aq			g/m3	1.25E-04	125.34
C_MeHg_2_Aq			g/m3	5.69E-06	5.69
C_Hg0_pore			g/m3	2.37E-05	23.73
C_HgII_pore			g/m3	1.08E-04	107.51
C_MeHg_pore			g/m3	1.32E-06	1.32
C_HgT_1_filtered			g/m3	1.65E-05	16.50
C_HgT_2_filtered			g/m3	1.55E-04	154.76
C_HgT_Sed_filtered			g/m3	1.33E-04	132.56
C_Hg0_1_T			g/m3	1.27E-05	12.65
C_HgII_1_T			g/m3	7.13E-05	71.27
C_MeHg_1_T			g/m3	2.66E-06	2.66
C_Hg0_2_T			g/m3	2.37E-05	23.73
C_HgII_2_T			g/m3	5.96E-04	595.89
C_MeHg_2_T			g/m3	8.50E-06	8.50
C_Hg0_sed			g/m3	1.97E-05	19.70
C_HgII_1_sed			g/m3	1.62E+01	16,159,539.54
C_MeHg_1_sed			g/m3	2.48E-02	24,811.24
C_Hg0_sed, wet			g/g	7.43E-12	0.00
C_HgII_1_sed, wet			g/g	1.26E-05	12.62
C_MeHg_1_sed, wet			g/g	2.97E-08	0.03
C_HgT_sed,wet			g/g	1.26E-05	12.65
C_Hg0_sed, dry weight			g/g	4.37E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.59E-05	35.87
C_MeHg_1_sed, dry weight			g/g	5.51E-08	0.06
C_HgT_1			g/m3	8.66E-05	86.58
C_HgT_2			g/m3	6.28E-04	628.13
C_HgT_Sed, dry weight			g/g	3.59E-05	35.93
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.07%	82.32%	14.61%
Layer 2			1.35%	94.87%	3.78%
Sediments			0.15%	99.85%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.81571%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	2.94813%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	3.61221%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.93402%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	14.62272%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	17.42109%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	55.71087%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{Hg1I} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{Hg1I}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{oIHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiaHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{oIMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abiaMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiaHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiaMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{sA} \cdot f^{w,2}_{abiaHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{sA} \cdot f^{w,2}_{abiaHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{sA} \cdot f^{w,2}_{abiaMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed	Matrix b		Solution Matrix
	1	2	3	4	5	6	7	8	9			
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	1.265E-05
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	7.127E-05
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T	2.657E-06
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	2.373E-05
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	5.959E-04
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T	8.504E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	1.970E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.62E+01	C_HgII_1_sed	1.616E+01
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed	2.481E-02

Inverted Matrix

										x=b/A
-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	1.27E-05	
-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	7.13E-05	
-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	2.66E-06	
-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	2.37E-05	
-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.000596	
-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	8.5E-06	
-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	1.97E-05	
8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	16.15954	
-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.024811	

Target C_sed, wet 16.18437048 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate cc	per yr	134.70
kw_v,HgII	water column volatilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatilization loss rate cc	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	122.63
kw_red_2	water column reduction rate constant,	per yr	23.27
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for I	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for I	per yr	0.82
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \Big/ \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{C_{diss,i}^j + C_{DOC,i}^j} = \frac{TSS}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.81571%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61221%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			2.94813%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93402%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			17.42109%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			14.62272%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.78562%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.16164%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00628%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.14683%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			73.17463%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.14319%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			73.80506%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			6.31498%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.99560%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.83
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	1.14
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	7,154.39
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3			
Sbio_phyto,1	5	TSS_1	8.46	mg/L
Sbio_zoo,1	2.5	TSS_2	1.34	mg/L
Sbio_phyto,2	0			
Sbio_zoo,2	0			
Sabio_1	1.34E-01			
Sabio_2	1.99E-01			
Sbio_dead,1	8.30E-01			
Sbio_dead,2	1.14E+00			
S_abio, sed	8.42E+04			
S_bio_dead,sed	7.15E+03			
S_sed,total	9.14E+04	g/m3		

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

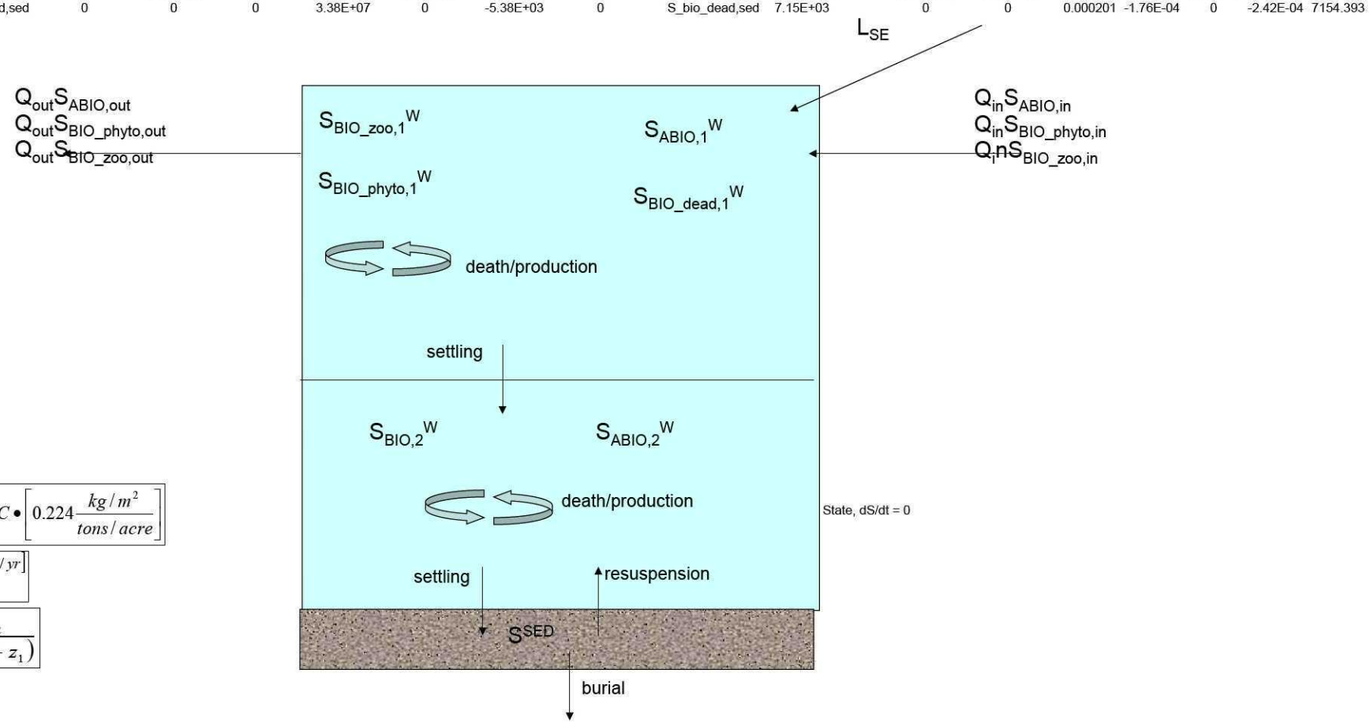
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	3.55E+07	S_bio_dead,1	8.30E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.829741
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	1.14E+00	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	1.138825
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	7.15E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	7154.393



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00816	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.03612		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03934		$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.17421		
k_meth_1	abiotic methylation in layer 1		per yr	3.46E-07		$k_{meth} = k_{meth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC}\right)$
k_meth_2	abiotic* methylation in layer 2		per yr	8.93E-06	if anoxic:	

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1	
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07		
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06		
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.16E-03		
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61E-02		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93E-02		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.74E-01		
k_demeth_1	biotic demethylation in layer 1		per yr	2.02E-07		$k_{demeth} = k_{demeth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC}\right)$
k_demeth_2	biotic demethylation in layer 2		per yr	8.93E-06		

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location	
East	YES
West	NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Belted Kingfisher Diet Comprised of 100% Trophic Level 3 Fish

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Kd_abio		
HgII	7,182,936	1
MeHg	15,887	1

Kd_bio		
HgII	17,941,378	1
MeHg	2,581,565	1

Kd_DOC		
HgII	301,427	1
MeHg	310,000	1
	PCT ERROR	CLEANUP
MeHg Filtered	9.50	7.44
HgT Filtered	-51.71	
MeHg Unfilte	-64.28	
HgT Unfiltere	-46.85	

Inflow Mercury Concentrations

Hg0	0	g/m3			
HgII	5.64E-06	g/m3	5.64	-38.33653462	
MeHg	7.33E-08	g/m3	0.07332	43.08721129	Fish

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27	ug/g	

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Exposure Concentrations

		Scenario 1 With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2 Background Conditions		Scenario 3 Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	11.73	ng/L		-11.73	-100	0.47	ng/L	2.79	ng/L
	HgII Filtered	3.14	ng/L		-3.14	-100	0.13	ng/L	0.75	ng/L
Epilimnion	MeHg Filtered	0.43	ng/L	0.47525	0.04	9.5013533	0.03	ng/L	0.11	ng/L
	HgT Filtered	15.31	ng/L	7.39	-7.92	-51.71183	0.63	ng/L	3.66	ng/L
	Hg0 Unfiltered	11.73	ng/L		-11.73	-100	0.47	ng/L	2.79	ng/L
	HgII Unfiltered	66.10	ng/L		-66.10	-100	2.67	ng/L	15.75	ng/L
	MeHg Unfiltered	2.47	ng/L	0.88225	-1.59	-64.28243	0.18	ng/L	0.65	ng/L
	HgT Unfiltered	80.30	ng/L	42.67625	-37.62	-46.85323	3.32	ng/L	19.20	ng/L
Hypolimnion	Hg0 Filtered	21.98	ng/L		-21.98	-100	0.53	ng/L	4.96	ng/L
	HgII Filtered	116.08	ng/L		-116.08	-100	2.59	ng/L	26.00	ng/L
	MeHg Filtered	5.28	ng/L		-5.28	-100	0.23	ng/L	1.27	ng/L
	HgT Filtered	143.34	ng/L		-143.34	-100	3.36	ng/L	32.23	ng/L
	Hg0 Unfiltered	21.98	ng/L		-21.98	-100	0.53	ng/L	4.96	ng/L
	HgII Unfiltered	551.86	ng/L		-551.86	-100	12.34	ng/L	123.60	ng/L
	MeHg Unfiltered	7.89	ng/L		-7.89	-100	0.35	ng/L	1.90	ng/L
	HgT Unfiltered	581.74	ng/L		-581.74	-100	13.21	ng/L	130.46	ng/L
	Sediment									
	Hg0 porewater	21.98	ng/L		-21.98	-100	0.53	ng/L	4.956	ng/L
	HgII porewater	99.56	ng/L		-99.56	-100	2.18	ng/L	22.266	ng/L
	MeHg porewater	1.22	ng/L		-1.22	-100	0.05	ng/L	0.289	ng/L
	HgT porewater	122.77	ng/L		-122.77	-100	2.76	ng/L	27.511	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.22	ug/g		-33.22	-100	0.39	ug/g	7.43	ug/g
	MeHg bulk, dry	0.05107	ug/g	0.00422	-0.05	-91.73681	0.00	ug/g	0.01	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.730	ug/g	7.44	ug/g
	Trophic Level 3	0.40	ug/g		-0.40	-100	0.029	ug/g	0.10	ug/g
	Trophic Level 4	0.86	ug/g		-0.86	-100	0.063	ug/g	0.23	ug/g
	HI	3.79					0.27		1.00	
	Sensitive Indicator	Kingfisher					Kingfisher		Kingfisher	
	Target C_sed, dry	7.44	ug/g	Note: 8						
	Target C_sed, wet	3.35	ug/g							

Rate Constants

Process	Media	Value	Units		
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		ratio Sed
1.00E-03	Sediment	3.49E-07	per day		Meth/demeth
Demethylation	Epilimnion	1.16E-08	per day		50.00%
1.00E-03	Hypolimnion	1.16E-07	per day		
2.00E-03	Sediment	6.98E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

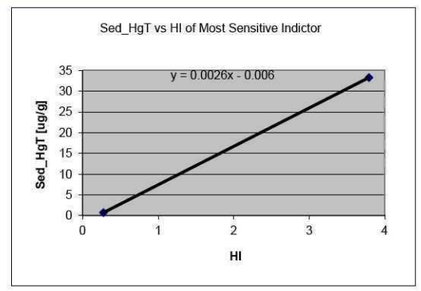
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed
Wildlife			Target-Level
Little Brown Bat	0.49	0.04	0.13
Otter	0.52	0.04	0.14
Mink	**1.02**	0.07	0.27
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.93	0.07	0.25
Kingfisher	**3.79**	0.27	**1.00**
Wood Duck	0.35	0.03	0.10
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
3.79	33.27
0.27	0.73
m =	9.256
b=	-1.815
Sed_HgT	7.441
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

	Site-Specific User Input	Required
	Model Calculated	No input required
	Data Necessary for certain sites	Only necessary if applicable to site of interest
	Scenario 1 Output	
	Scenario 2 Output	
	Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.43	0.03	0.114	ng/L

Biota

Trophic Level 1: Phytoplankton	0.08	0.01	0.02	ug Hg/ g wet weight
Trophic Level 2: Insects	0.07	0.01	0.02	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.02	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.40	0.03	0.10	ug Hg/ g wet weight
Trophic Level 4: Bass	0.86	0.06	0.23	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.47	0.03	0.12	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.08	0.01	0.02	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.02	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + (drinking\ rate \bullet [Hg]_{water})$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Body Weight	Ingestion Rate	Drinking rate	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants	Percent of Diet from Trophic Level 2 : Insects	Percent of Diet from Trophic Level 2 : Crayfish or Frogs	Percent of Diet from Trophic Level 3 : Fish	Percent of Diet from Trophic Level 4 : Fish	Percent of Diet from nonaquatic sources	Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Insects	Potential Dose from Trophic Level 2: Crayfish	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
Animal	[kg in wet weight]	[kg wet weight/d]	[L/d]	--	--	--	--	--	--	[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	36	0	0	0	36	75	0.49
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	29	9	39	75	0.52
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	70	76	75	1.02
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	18	6	32	0	56	60	0.93
Kingfisher	0.15	0.086	0.017	0%	0%	0%	100%	0%	0%	0	0	0	0	227	0	227	60	3.79
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	17	5	0	0	0	22	60	0.36
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	8	5000	0.00
Human																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Wildlife Specific Parameters | **Contaminated Sediment Calculations** | **Human Specific Parameters**

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Belted Kingfigher - Diet Comprised of 100% Trophic Level 2 Fish

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.005	0.00	2.64	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.08	2.14	0.62	3	75	0.04
0.003	0.00	0.00	0.27	0.19	5.06	6	75	0.07
0.001	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.015	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.002	0.00	1.27	0.46	2.32	0.00	4	60	0.07
0.004	0.00	0.00	0.00	16.50	0.00	16	60	0.27
0.002	1.22	0.36	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.03	0.08	0.48	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.018	0.00	9.61	0.00	0.00	0.00	10	75	0.13
0.010	0.00	0.00	0.31	7.77	2.26	10	75	0.14
0.011	0.00	0.00	0.97	0.70	18.42	20	75	0.27
0.005	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.054	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.008	0.00	4.62	1.66	8.43	0.00	15	60	0.25
0.013	0.00	0.00	0.00	60.00	0.00	60	60	**1.00**
0.008	4.42	1.30	0.00	0.00	0.00	6	60	0.10
0.000	0.00	0.00	0.12	0.28	1.75	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Coun	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeHg	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and reflec		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

this table does not all correspond to EPA Report to Congress - check!

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	
HgII	Mean	58,000	50000	100,000	200,000	
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000		
MeHg	Mean	7000	3000	100,000	500,000	
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000		
Hg0		1,000	1,000	3000	1,000	NTG added these 11/1/19

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.71E-07	0.47
C_HgII_1_Aq			g/m3	1.27E-07	0.13
C_MeHg_1_Aq			g/m3	3.15E-08	0.03
C_Hg0_2_Aq			g/m3	5.32E-07	0.53
C_HgII_2_Aq			g/m3	2.59E-06	2.59
C_MeHg_2_Aq			g/m3	2.31E-07	0.23
C_Hg0_pore			g/m3	5.32E-07	0.53
C_HgII_pore			g/m3	2.18E-06	2.18
C_MeHg_pore			g/m3	4.76E-08	0.05
C_HgT_1_filtered			g/m3	6.30E-07	0.63
C_HgT_2_filtered			g/m3	3.36E-06	3.36
C_HgT_Sed_filtered			g/m3	2.76E-06	2.76
C_Hg0_1_T			g/m3	4.71E-07	0.47
C_HgII_1_T			g/m3	2.67E-06	2.67
C_MeHg_1_T			g/m3	1.79E-07	0.18
C_Hg0_2_T			g/m3	5.32E-07	0.53
C_HgII_2_T			g/m3	1.23E-05	12.34
C_MeHg_2_T			g/m3	3.45E-07	0.35
C_Hg0_sed_bulk			g/m3	4.42E-07	0
C_HgII_1_sed_bulk			g/m3	3.28E-01	328.097
C_MeHg_1_sed_bulk			g/m3	8.97E-04	897
C_Hg0_sed_wet			g/g	3.45E-13	0.000
C_HgII_1_sed_wet			g/g	3.93E-07	0.393
C_MeHg_1_sed_wet			g/g	6.65E-14	0.000
C_HgT_sed,wet			g/g	3.93E-07	0.393
C_Hg0_sed_dry weight			g/g	9.80E-13	0.0000
C_HgII_1_sed_dry weight			g/g	7.28E-07	0.7283
C_MeHg_1_sed_dry weight			g/g	1.99E-09	0.0020
C_HgT_1			g/m3	3.32E-06	3.321
C_HgT_2			g/m3	1.32E-05	13.213
C_HgT_Sed, dry weight			g/g	7.30E-07	0.730

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)	5.40%	80.41%	14.19%
Layer 2		2.61%	93.36%	4.03%
Sediments		0.27%	99.73%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V_1	Volume of Layer 1	Aw*z_1	m3	648,711
V_2	Volume of Layer 2	Aw*z_2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.008
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.029
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.036
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.112
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.039
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.146
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.174
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.557

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{d C^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[k w_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[k w_{mer} \cdot V_w + k w_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - k w_{volHg0} \cdot V_w - k w_{vsid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiotHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{d C^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[k w_{sid} V_w\right] \cdot C^w_{Hg0,1} + \left[k w_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - k w_{volHgII} V_w - k w_{red1} \cdot V_w - k w_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abiotHgII} A_w - v_{sB} \cdot f^{w,1}_{biotHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{d C^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[k w_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - k w_{volMeHg} V_w - k w_{demeth} \cdot V_w - k w_{mer} \cdot V_w - k w_{photorhd} V_w - v_{sA} \cdot f^{w,1}_{abiotMeHg} A_w - v_{sB} \cdot f^{w,1}_{biotMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{d C^w_{Hg0,2}}{dt} = +\left[k w_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[k w_{mer} \cdot V_w + k w_{photorhd} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - k w_{vsid} V_w - v_{sA} \cdot f^{w,2}_{abiotHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot A_w \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{d C^w_{HgII2}}{dt} = +\left[k w_{vsid} V_w\right] \cdot C^w_{Hg0,2} + \left[k w_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - k w_{red2} \cdot V_w - k w_{meth2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiotHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{d C^w_{MeHg2}}{dt} = +\left[k w_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - k w_{demeth2} \cdot V_w - k w_{mer} \cdot V_w - k w_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{d C^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - k b_{vsid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[k b_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[k b_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{d C^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abiotHgII} + v_{sB} \cdot f^{w,2}_{biotHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[k b_{vsid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(k b_{red} + k b_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[k b_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{d C^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[k b_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(k b_{demeth} + k b_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E+08	0.00E+00	0.00E+00	-5.25E+03	3.54E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03

A*x=b

Matrix b

C_Hg0_1_T	-4.89E-01
C_HgII_1_T	-6.18E+01
C_MeHg_1_T	-1.43E+00
C_Hg0_2_T	0.00E+00
C_HgII_2_T	0.00E+00
C_MeHg_2_T	0.00E+00
C_Hg0_sed	0.00E+00
C_HgII_1_sed	0.00E+00
C_MeHg_1_sed	0.00E+00

Solution Matrix (x=b/A)

	Inverted Matrix									
C_Hg0_1_T	4.712E-07	-8.13E-09	-7.48E-09	-3.10E-09	-7.60E-09	-7.47E-09	-3.13E-09	-7.60E-09	-7.47E-09	-3.14E-09	4.71217E-07
C_HgII_1_T	2.670E-06	-3.39E-08	-4.26E-08	-1.30E-08	-4.05E-08	-4.21E-08	-1.32E-08	-4.05E-08	-4.21E-08	-1.32E-08	2.67016E-06
C_MeHg_1_T	1.792E-07	-6.58E-10	-8.19E-10	-8.94E-08	-1.33E-09	-1.49E-09	-8.87E-08	-1.33E-09	-1.52E-09	-8.86E-08	1.79194E-07
C_Hg0_2_T	5.321E-07	-7.220E-09	-8.479E-09	-2.945E-09	-4.60E-08	-1.42E-08	-3.24E-09	-4.60E-08	-1.42E-08	-3.25E-09	5.3214E-07
C_HgII_2_T	1.234E-05	-1.581E-07	-1.968E-07	-6.130E-08	-3.19E-07	-3.58E-07	-6.34E-08	-3.19E-07	-3.58E-07	-6.36E-08	1.23359E-05
C_MeHg_2_T	3.452E-07	-2.166E-09	-2.697E-09	-1.236E-07	-4.38E-09	-4.91E-09	-2.92E-07	-4.38E-09	-5.00E-09	-2.92E-07	3.45194E-07
C_Hg0_sed	4.417E-07	-5.99E-09	-7.04E-09	-2.44E-09	-3.82E-08	-1.18E-08	-2.69E-09	-3.24E-06	-1.18E-08	-2.69E-09	4.41677E-07
C_HgII_1_sed	3.281E-01	-4.20E-03	-5.23E-03	-1.63E-03	-8.49E-03	-9.52E-03	-1.69E-03	-8.49E-03	-9.71E-03	-1.69E-03	0.328097232
C_MeHg_1_sed	8.968E-04	-6.35E-06	-7.91E-06	-2.82E-04	-1.28E-05	-1.44E-05	-6.66E-04	-1.28E-05	-1.47E-05	-8.55E-04	0.000896776

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.008
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.052
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.091
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.732
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.121
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.063
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.738
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.330
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		5.52E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		4.40E-05
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methv	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2]\left[H^+\right]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} = \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS} = \frac{C_{filtered,i}^{j}}{C_{diss,i}^{j}+C_{DOC,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.17E-05	11.73
C_HgII_1_Aq			g/m3	3.14E-06	3.14
C_MeHg_1_Aq			g/m3	4.34E-07	0.43
C_Hg0_2_Aq			g/m3	2.20E-05	21.98
C_HgII_2_Aq			g/m3	1.16E-04	116.08
C_MeHg_2_Aq			g/m3	5.28E-06	5.28
C_Hg0_pore			g/m3	2.20E-05	21.98
C_HgII_pore			g/m3	9.96E-05	99.56
C_MeHg_pore			g/m3	1.22E-06	1.22
C_HgT_1_filtered			g/m3	1.53E-05	15.31
C_HgT_2_filtered			g/m3	1.43E-04	143.34
C_HgT_Sed_filtered			g/m3	1.23E-04	122.77
C_Hg0_1_T			g/m3	1.17E-05	11.73
C_HgII_1_T			g/m3	6.61E-05	66.10
C_MeHg_1_T			g/m3	2.47E-06	2.47
C_Hg0_2_T			g/m3	2.20E-05	21.98
C_HgII_2_T			g/m3	5.52E-04	551.86
C_MeHg_2_T			g/m3	7.89E-06	7.89
C_Hg0_sed			g/m3	1.82E-05	18.25
C_HgII_1_sed			g/m3	1.50E+01	14965109.78
C_MeHg_1_sed			g/m3	2.30E-02	23006.97
C_Hg0_sed, wet			g/g	6.89E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.687
C_MeHg_1_sed, wet			g/g	2.75E-08	0.028
C_HgT_sed,wet			g/g	1.17E-05	11.714
C_Hg0_sed, dry weight			g/g	4.05E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.32E-05	33.22
C_MeHg_1_sed, dry weight			g/g	5.11E-08	0.05
C_HgT_1			g/m3	8.03E-05	80.30
C_HgT_2			g/m3	5.82E-04	581.74
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.08%	82.31%	14.61%
Layer 2			1.36%	94.86%	3.78%
Sediments			0.15%	99.85%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.81571%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	2.94813%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	3.61221%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.93402%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	14.62272%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	17.42109%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03550%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red,1} \cdot V_w - kw_{metlR} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg1}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{metlR} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg1} + Q' \cdot C^w_{MeHg2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abiHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{red2} \cdot V_w - kw_{metlR} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{metlR} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2} + Q' \cdot C^w_{MeHg3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix											x=b/A
1.173E-05	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	1.17E-05	C_Hg0_1_T	
6.610E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	6.61E-05	C_HgII_1_T	
2.470E-06	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	2.47E-06	C_MeHg_1_T	
2.198E-05	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	2.2E-05	C_Hg0_2_T	
5.519E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.000552	C_HgII_2_T	
7.888E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	7.89E-06	C_MeHg_2_T	
1.825E-05	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	1.82E-05	C_Hg0_sed	
1.497E+01	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	14.96511	C_HgII_1_sed	
2.301E-02	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.023007	C_MeHg_1_sed	

A*x=b

C_T_sed 14.988135 g/m3

$$C^{sed}_{dry.}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	13900.95
TSS_1			mg/L	8.46
TSS+2			mg/L	1.34
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_Hg0_1	Effective K for Hg0 in layer 2		L/kg	2.37E+06
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.54E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	3.69E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	2.79E-06	2.79
C_HgII_1_Aq			g/m3	7.48E-07	0.75
C_MeHg_1_Aq			g/m3	1.14E-07	0.11
C_Hg0_2_Aq			g/m3	4.96E-06	4.96
C_HgII_2_Aq			g/m3	2.60E-05	26.00
C_MeHg_2_Aq			g/m3	1.27E-06	1.27
C_Hg0_pore			g/m3	4.96E-06	4.96
C_HgII_pore			g/m3	2.23E-05	22.27
C_MeHg_pore			g/m3	2.89E-07	0.29
C_HgT_1_filtered			g/m3	3.66E-06	3.66
C_HgT_2_filtered			g/m3	3.22E-05	32.23
C_HgT_Sed_filtered			g/m3	2.75E-05	27.51
C_Hg0_1_T			g/m3	2.79E-06	2.79
C_HgII_1_T			g/m3	1.58E-05	15.75
C_MeHg_1_T			g/m3	6.52E-07	0.65
C_Hg0_2_T			g/m3	4.96E-06	4.96
C_HgII_2_T			g/m3	1.24E-04	123.60
C_MeHg_2_T			g/m3	1.90E-06	1.90
C_Hg0_sed			g/m3	4.11E-06	4.11
C_HgII_1_sed			g/m3	3.35E+00	3,346,648.33
C_MeHg_1_sed			g/m3	5.46E-03	5,456.50
C_Hg0_sed, wet			g/g	1.55E-12	0.00
C_HgII_1_sed, wet			g/g	2.61E-06	2.61
C_MeHg_1_sed, wet			g/g	6.53E-09	0.01
C_HgT_sed,wet			g/g	2.62E-06	2.62
C_Hg0_sed, dry weight			g/g	9.13E-12	0.00
C_HgII_1_sed, dry weight			g/g	7.43E-06	7.43
C_MeHg_1_sed, dry weight			g/g	1.21E-08	0.01
C_HgT_1			g/m3	1.92E-05	19.20
C_HgT_2			g/m3	1.30E-04	130.46
C_HgT_Sed, dry weight			g/g	7.44E-06	7.44
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.39%	82.05%	14.55%
Layer 2			1.46%	94.74%	3.80%
Sediments			0.16%	99.84%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.81571%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			2.94813%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61221%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			11.23203%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			3.93402%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			14.62272%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			17.42109%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			55.71087%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot A_w \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	2.794E-06	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	2.8E-06
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	1.575E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	1.6E-05
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T	6.516E-07	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	6.5E-07
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	4.956E-06	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	5E-06
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	1.236E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.00012
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T	1.901E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	1.9E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	4.114E-06	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	4.1E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	3.35E+00	C_HgII_1_sed	3.347E+00	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	3.34665
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed	5.457E-03	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.00546

A*x=b

Target C_sed, wet 3.352108948 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	134.70
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.22
kw_oxd_1	water column oxidation rate constant	per yr	554.95
kw_oxd_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	122.63
kw_red_2	water column reduction rate constant	per yr	23.27
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for	per yr	0.82
kw_mer	water column *mer* cleavage demethy	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeH	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\ \frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \times 10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \Big/ \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{C_{filtered,i}^j}{C_{diss,i}^j + C_{DOC,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.81571%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61221%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			2.94813%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93402%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			17.42109%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			14.62272%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.78562%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.16164%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00628%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.14683%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			73.17463%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.14319%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			73.80506%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			6.31498%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.99560%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.83
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	1.14
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	7,154.39
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed}+K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6}+K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	8.46	mg/L
Sbio_zoo,1	2.5		TSS_2	1.34	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	8.30E-01				
Sbio_dead,2	1.14E+00				
S_abio, sed	8.42E+04				
S_bio_dead,sed	7.15E+03				
S_sed,total	9.14E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

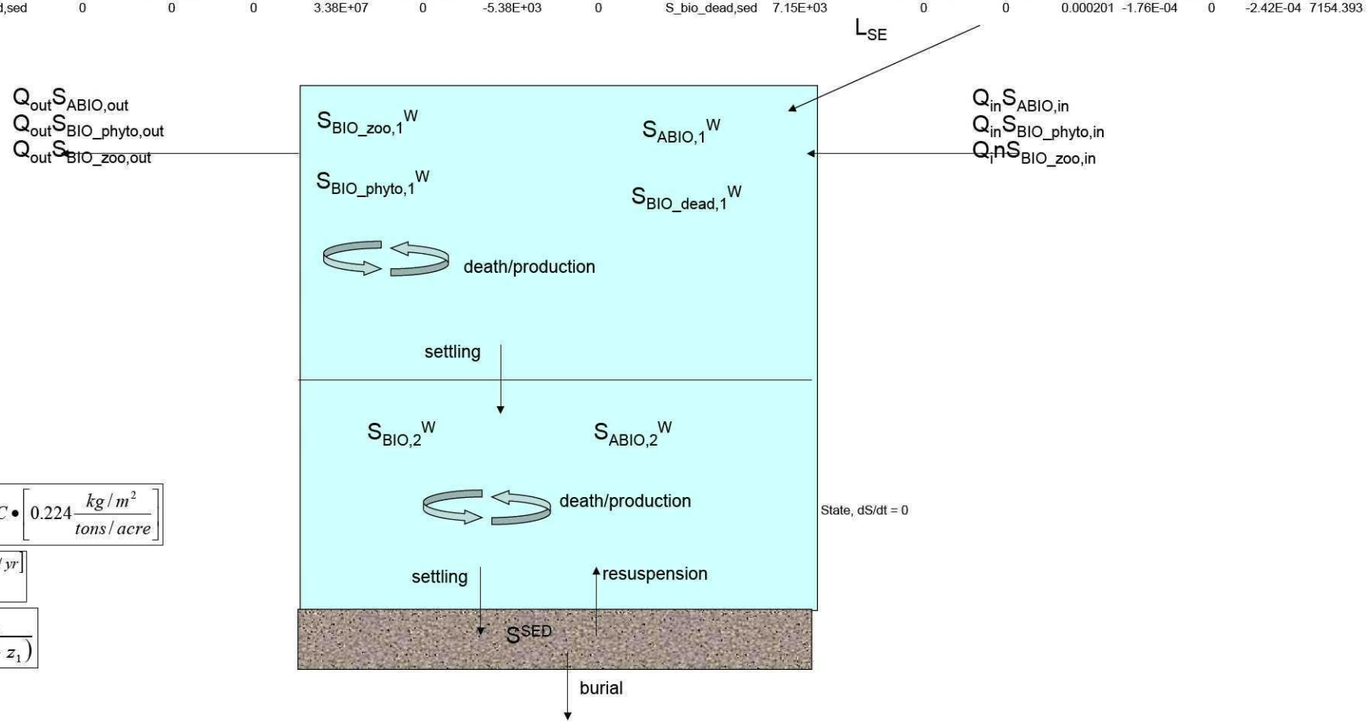
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	3.55E+07	S_bio_dead,1	8.30E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.829741
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	1.14E+00	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	1.138825
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	7.15E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	7154.393



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00816	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.03612		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03934		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.17421		
k_meth_1	abiotic methylation in layer 1		per yr	3.46E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	8.93E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.16E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.74E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.02E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	8.93E-06	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

1 UV-B is modeled as being 0.5% of visible light.
check?

1 $$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Belted Kingfisher - Diet Comprised of 100% Trophic Level 3 Fish

Location	
East	YES
West	NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Belted Kingfisher – Varied Diet

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	-38.33653462
MeHg	7.33E-08	g/m3	0.07332	43.08721129

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27	ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3
Cs,HgII	1.129080624	g/m3
Cs,MeHg	4.13E-03	g/m3

Required Hazard Index for Sensitive Indicator	1

Kd_abio			
HgII	7,182,936	1	
MeHg	15,887	1	
Kd_bio			
HgII	17,941,378	1	
MeHg	2,581,565	1	
Kd_DOC			
HgII	301,427	1	
MeHg	310,000	1	
	PCT ERROR	CLEANUP	
MeHg Filtered	9.50	17.58	
HgT Filtered	-51.71		
MeHg Unfilter	-64.28		
HgT Unfiltere	-46.85		

Exposure Concentrations

		Scenario 1 With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2 Background Conditions		Scenario 3 Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	11.73	ng/L		-11.73	-100	0.47	ng/L	6.30	ng/L
	HgII Filtered	3.14	ng/L		-3.14	-100	0.13	ng/L	1.69	ng/L
Epilimnion	MeHg Filtered	0.43	ng/L	0.47525	0.04	9.5013533	0.03	ng/L	0.24	ng/L
	HgT Filtered	15.31	ng/L	7.39	-7.92	-51.71183	0.63	ng/L	8.23	ng/L
	Hg0 Unfiltered	11.73	ng/L		-11.73	-100	0.47	ng/L	6.30	ng/L
	HgII Unfiltered	66.10	ng/L		-66.10	-100	2.67	ng/L	35.52	ng/L
	MeHg Unfiltered	2.47	ng/L	0.88225	-1.59	-64.28243	0.18	ng/L	1.37	ng/L
	HgT Unfiltered	80.30	ng/L	42.67625	-37.62	-46.85323	3.32	ng/L	43.19	ng/L
Hypolimnion	Hg0 Filtered	21.98	ng/L		-21.98	-100	0.53	ng/L	11.64	ng/L
	HgII Filtered	116.08	ng/L		-116.08	-100	2.59	ng/L	61.36	ng/L
	MeHg Filtered	5.28	ng/L		-5.28	-100	0.23	ng/L	2.85	ng/L
	HgT Filtered	143.34	ng/L		-143.34	-100	3.36	ng/L	75.85	ng/L
	Hg0 Unfiltered	21.98	ng/L		-21.98	-100	0.53	ng/L	11.64	ng/L
	HgII Unfiltered	551.86	ng/L		-551.86	-100	12.34	ng/L	291.74	ng/L
	MeHg Unfiltered	7.89	ng/L		-7.89	-100	0.35	ng/L	4.25	ng/L
	HgT Unfiltered	581.74	ng/L		-581.74	-100	13.21	ng/L	307.63	ng/L
	Sediment									
	Hg0 porewater	21.98	ng/L		-21.98	-100	0.53	ng/L	11.641	ng/L
	HgII porewater	99.56	ng/L		-99.56	-100	2.18	ng/L	52.614	ng/L
	MeHg porewater	1.22	ng/L		-1.22	-100	0.05	ng/L	0.655	ng/L
	HgT porewater	122.77	ng/L		-122.77	-100	2.76	ng/L	64.910	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.22	ug/g		-33.22	-100	0.39	ug/g	17.55	ug/g
	MeHg bulk, dry	0.05107	ug/g	0.00422	-0.05	-91.73681	0.00	ug/g	0.03	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.730	ug/g	17.58	ug/g
Fish	Trophic Level 3	0.40	ug/g		-0.40	-100	0.029	ug/g	0.22	ug/g
	Trophic Level 4	0.86	ug/g		-0.86	-100	0.063	ug/g	0.48	ug/g
	HI	1.81					0.13		1.00	
	Sensitive Indicator	Kingfisher					Kingfisher		Kingfisher	
	Target C_sed, dry	17.58	ug/g	Note: 8						
	Target C_sed, wet	7.92	ug/g							

Rate Constants

Process	Media	Value	Units		
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		ratio Sed
1.00E-03	Sediment	3.49E-07	per day		Meth/demeth
Demethylation	Epilimnion	1.16E-08	per day		50.00%
1.00E-03	Hypolimnion	1.16E-07	per day		
2.00E-03	Sediment	6.98E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

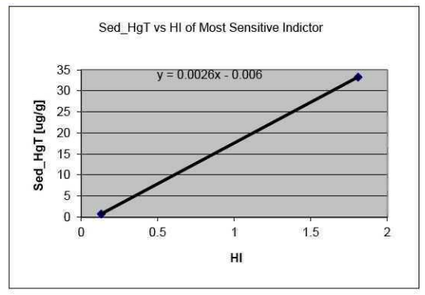
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.49	0.04	0.27
Otter	0.52	0.04	0.29
Mink	**1.02**	0.07	0.56
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.93	0.07	0.51
Kingfisher	**1.81**	0.13	**1.00**
Wood Duck	0.36	0.03	0.20
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
1.81	33.27
0.13	0.73
m =	19.397
b=	-1.815
Sed_HgT	17.582
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.43	0.03	0.240	ng/L

Biota

Trophic Level 1: Phytoplankton	0.08	0.01	0.05	ug Hg/ g wet weight
Trophic Level 2: Insects	0.07	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.40	0.03	0.22	ug Hg/ g wet weight
Trophic Level 4: Bass	0.86	0.06	0.48	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.47	0.03	0.26	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.04	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

	Wildlife Specific Parameters									Contaminated Sediment Calculations								
Animal	**Body Weight** [kg in wet weight]	**Ingestion Rate** [kg wet weight/d]	**Drinking rate** [L/d]	**Percent of Diet from Trophic Level 1 : Phytoplankton and Plants** --	**Percent of Diet from Trophic Level 2 : Insects** --	**Percent of Diet from Trophic Level 2 : Crayfish or Frogs** --	**Percent of Diet from Trophic Level 3 : Fish** --	**Percent of Diet from Trophic Level 4 : Fish** --	**Percent of Diet from nonaquatic sources** --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	36	0	0	0	36	75	0.49
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	29	9	39	75	0.52
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	70	76	75	**1.02**
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	18	6	32	0	56	60	0.93
Kingfisher	0.15	0.086	0.017	0%	0%	18%	23%	10%	50%	0	0	0	8	51	50	109	60	**1.81**
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	17	5	0	0	0	22	60	0.36
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	8	5000	0.00
Human	**Human Specific Parameters**																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.005	0.00	2.64	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.08	2.14	0.62	3	75	0.04
0.003	0.00	0.00	0.27	0.19	5.06	6	75	0.07
0.001	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.015	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.002	0.00	1.27	0.46	2.32	0.00	4	60	0.07
0.004	0.00	0.00	0.57	3.71	3.59	8	60	0.13
0.002	1.22	0.36	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.03	0.08	0.48	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.038	0.00	20.14	0.00	0.00	0.00	20	75	0.27
0.020	0.00	0.00	0.64	16.29	4.73	22	75	0.29
0.024	0.00	0.00	2.04	1.48	38.59	42	75	0.56
0.011	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.113	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.017	0.00	9.69	3.48	17.67	0.00	31	60	0.51
0.027	0.00	0.00	4.33	28.29	27.38	60	60	**1.00**
0.016	9.27	2.73	0.00	0.00	0.00	12	60	0.20
0.000	0.00	0.00	0.24	0.60	3.66	4	5000	0.00
							RfD	
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.71E-07	0.47
C_HgII_1_Aq			g/m3	1.27E-07	0.13
C_MeHg_1_Aq			g/m3	3.15E-08	0.03
C_Hg0_2_Aq			g/m3	5.32E-07	0.53
C_HgII_2_Aq			g/m3	2.59E-06	2.59
C_MeHg_2_Aq			g/m3	2.31E-07	0.23
C_Hg0_pore			g/m3	5.32E-07	0.53
C_HgII_pore			g/m3	2.18E-06	2.18
C_MeHg_pore			g/m3	4.76E-08	0.05
C_HgT_1_filtered			g/m3	6.30E-07	0.63
C_HgT_2_filtered			g/m3	3.36E-06	3.36
C_HgT_Sed_filtered			g/m3	2.76E-06	2.76
C_Hg0_1_T			g/m3	4.71E-07	0.47
C_HgII_1_T			g/m3	2.67E-06	2.67
C_MeHg_1_T			g/m3	1.79E-07	0.18
C_Hg0_2_T			g/m3	5.32E-07	0.53
C_HgII_2_T			g/m3	1.23E-05	12.34
C_MeHg_2_T			g/m3	3.45E-07	0.35
C_Hg0_sed, bulk			g/m3	4.42E-07	0
C_HgII_1_sed, bulk			g/m3	3.28E-01	328,097
C_MeHg_1_sed, bulk			g/m3	8.97E-04	897
C_Hg0_sed, wet			g/g	3.45E-13	0.000
C_HgII_1_sed, wet			g/g	3.93E-07	0.393
C_MeHg_1_sed, wet			g/g	6.65E-14	0.000
C_HgT_sed,wet			g/g	3.93E-07	0.393
C_Hg0_sed, dry weight			g/g	9.80E-13	0.0000
C_HgII_1_sed, dry weight			g/g	7.28E-07	0.7283
C_MeHg_1_sed, dry weight			g/g	1.99E-09	0.0020
C_HgT_1			g/m3	3.32E-06	3.321
C_HgT_2			g/m3	1.32E-05	13.213
C_HgT_Sed, dry weight			g/g	7.30E-07	0.730

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)	5.40%	80.41%	14.19%
Layer 2		2.61%	93.36%	4.03%
Sediments		0.27%	99.73%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V_1	Volume of Layer 1	Aw*z_1	m3	648,711
V_2	Volume of Layer 2	Aw*z_2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.008
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.029
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.036
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.112
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.039
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.146
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.174
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.557

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{s,B} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxi} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHgII} A_w - v_{s,B} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s,A} \cdot f^{w,1}_{abioMeHg} A_w - v_{s,B} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red,2} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioHgII} A_w - v_{s,B} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{s,B} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,A} \cdot f^{w,2}_{abioHg0} + v_{s,B} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sed,Hg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,A} \cdot f^{w,2}_{abioHgII} + v_{s,B} \cdot f^{w,2}_{bioHgII}\right) A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,A} \cdot f^{w,2}_{abioMeHg} + v_{s,B} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sed,MeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C Hg0 1 T	C HgII 1 T	C MeHg 1 T	C Hg0 2 T	C HgII 2 T	C MeHg 2 T	C Hg0 1 sed	C HgII 1 sed	C MeHg 1 sed
	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E+08	0.00E+00	0.00E+00	-5.25E+03	3.54E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03

A*x=b

Matrix b	
C Hg0 1 T	-4.89E-01
C HgII 1 T	-6.18E+01
C MeHg 1 T	-1.43E+00
C Hg0 2 T	0.00E+00
C HgII 2 T	0.00E+00
C MeHg 2 T	0.00E+00
C Hg0 sed	0.00E+00
C HgII 1 sed	0.00E+00
C MeHg 1 sed	0.00E+00

Solution Matrix	
C Hg0 1 T	4.712E-07
C HgII 1 T	2.670E-06
C MeHg 1 T	1.792E-07
C Hg0 2 T	5.321E-07
C HgII 2 T	1.234E-05
C MeHg 2 T	3.452E-07
C Hg0 sed	4.417E-07
C HgII 1 sed	3.281E-01
C MeHg 1 sed	8.968E-04

Inverted Matrix

-8.13E-09	-7.48E-09	-3.10E-09	-7.60E-09	-7.47E-09	-3.13E-09	-7.60E-09	-7.47E-09	-3.14E-09	4.71217E-07
-3.39E-08	-4.26E-08	-1.30E-08	-4.05E-08	-4.21E-08	-1.32E-08	-4.05E-08	-4.21E-08	-1.32E-08	2.67016E-06
-6.58E-10	-8.19E-10	-8.94E-08	-1.33E-09	-1.49E-09	-8.87E-08	-1.33E-09	-1.52E-09	-8.86E-08	1.79194E-07
-7.220E-09	-8.479E-09	-2.945E-09	-4.60E-08	-1.42E-08	-3.24E-09	-4.60E-08	-1.42E-08	-3.25E-09	5.3214E-07
-1.581E-07	-1.968E-07	-6.130E-08	-3.19E-07	-3.58E-07	-6.34E-08	-3.19E-07	-3.58E-07	-6.36E-08	1.23359E-05
-2.166E-09	-2.697E-09	-1.236E-07	-4.38E-09	-4.91E-09	-2.92E-07	-4.38E-09	-5.00E-09	-2.92E-07	3.45194E-07
-5.99E-09	-7.04E-09	-2.44E-09	-3.82E-08	-1.18E-08	-2.69E-09	-3.24E-06	-1.18E-08	-2.69E-09	4.41677E-07
-4.20E-03	-5.23E-03	-1.63E-03	-8.49E-03	-9.52E-03	-1.69E-03	-8.49E-03	-9.71E-03	-1.69E-03	0.328097232
-6.35E-06	-7.91E-06	-2.82E-04	-1.28E-05	-1.44E-05	-6.66E-04	-1.28E-05	-1.47E-05	-8.55E-04	0.000896776

x=b/A

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Belted Kingfisher – Varied Diet

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.008
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.052
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.091
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.732
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.121
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.063
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.738
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.330
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		5.52E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		4.40E-05
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org,i}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}} \quad \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.17E-05	11.73
C_HgII_1_Aq			g/m3	3.14E-06	3.14
C_MeHg_1_Aq			g/m3	4.34E-07	0.43
C_Hg0_2_Aq			g/m3	2.20E-05	21.98
C_HgII_2_Aq			g/m3	1.16E-04	116.08
C_MeHg_2_Aq			g/m3	5.28E-06	5.28
C_Hg0_pore			g/m3	2.20E-05	21.98
C_HgII_pore			g/m3	9.96E-05	99.56
C_MeHg_pore			g/m3	1.22E-06	1.22
C_HgT_1_filtered			g/m3	1.53E-05	15.31
C_HgT_2_filtered			g/m3	1.43E-04	143.34
C_HgT_Sed_filtered			g/m3	1.23E-04	122.77
C_Hg0_1_T			g/m3	1.17E-05	11.73
C_HgII_1_T			g/m3	6.61E-05	66.10
C_MeHg_1_T			g/m3	2.47E-06	2.47
C_Hg0_2_T			g/m3	2.20E-05	21.98
C_HgII_2_T			g/m3	5.52E-04	551.86
C_MeHg_2_T			g/m3	7.89E-06	7.89
C_Hg0_sed			g/m3	1.82E-05	18.25
C_HgII_1_sed			g/m3	1.50E+01	14965109.78
C_MeHg_1_sed			g/m3	2.30E-02	23006.97
C_Hg0_sed, wet			g/g	6.89E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.687
C_MeHg_1_sed, wet			g/g	2.75E-08	0.028
C_HgT_sed,wet			g/g	1.17E-05	11.714
C_Hg0_sed, dry weight			g/g	4.05E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.32E-05	33.22
C_MeHg_1_sed, dry weight			g/g	5.11E-08	0.05
C_HgT_1			g/m3	8.03E-05	80.30
C_HgT_2			g/m3	5.82E-04	581.74
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.08%	82.31%	14.61%
Layer 2			1.36%	94.86%	3.78%
Sediments			0.15%	99.85%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.81571%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	2.94813%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	3.61221%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.93402%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	14.62272%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	17.42109%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03550%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{vol Hg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{metR} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg1}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{metB} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg1} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{red2} \cdot V_w - kw_{metR} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{metB2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2} + Q' \cdot C^w_{MeHg1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w}{\theta_{sed}}\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2) from Mortimer, cited in Schnoor, 1996, pg. 57. for rivers, this will be different (see Schnoor)

Matrix A

	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix

1.173E-05
6.610E-05
2.470E-06
2.198E-05
5.519E-04
7.888E-06
1.825E-05
1.497E+01
2.301E-02

Inverted Matrix

-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	1.17E-05
-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	6.61E-05
-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	2.47E-06
-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	2.2E-05
-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.000552
-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	7.89E-06
-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	1.82E-05
8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	14.96511
-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.023007

x=b/A

A*x=b

C T sed 14.988135 g/m3

$$C^{sed}_{dry.}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity		m/yr		4792.628412
v_sB	biotic settling velocity		m/yr		73
v_rs	resuspension velocity		m/yr		0.003700005
k_mort	phytoplankton mortality rate		per yr		10.95
v_min	mineralization rate		per yr		0.01
v_bur	burial rate		m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0			m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII			m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg			m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0			m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII			m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg			m2/sec	6.11E-10
rho_s	Sediment Particle Density			g/cm3	2.65E+00
θ_sed	sediment porosity			cm3/cm3	0.83
z_sed	sediment layer,char mixing length			m	0.03
V_sed	Volume of Sediment	Aw*z_sed		m3	13900.95
TSS_1				mg/L	8.46
TSS+2				mg/L	1.34
Effective Partition Coefficients for each Hg species and layer					
K_eff_Hg0_1	Effective K for Hg0 in layer 1			L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2			L/kg	2.37E+06
K_eff_MeHg_1	Effective K for HgII in layer 1			L/kg	5.54E+05
K_eff_Hg0_2	Effective K for HgII in layer 2			L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1			L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2			L/kg	3.69E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	6.30E-06	6.30
C_HgII_1_Aq			g/m3	1.69E-06	1.69
C_MeHg_1_Aq			g/m3	2.40E-07	0.24
C_Hg0_2_Aq			g/m3	1.16E-05	11.64
C_HgII_2_Aq			g/m3	6.14E-05	61.36
C_MeHg_2_Aq			g/m3	2.85E-06	2.85
C_Hg0_pore			g/m3	1.16E-05	11.64
C_HgII_pore			g/m3	5.26E-05	52.61
C_MeHg_pore			g/m3	6.55E-07	0.65
C_HgT_1_filtered			g/m3	8.23E-06	8.23
C_HgT_2_filtered			g/m3	7.59E-05	75.85
C_HgT_Sed_filtered			g/m3	6.49E-05	64.91
C_Hg0_1_T			g/m3	6.30E-06	6.30
C_HgII_1_T			g/m3	3.55E-05	35.52
C_MeHg_1_T			g/m3	1.37E-06	1.37
C_Hg0_2_T			g/m3	1.16E-05	11.64
C_HgII_2_T			g/m3	2.92E-04	291.74
C_MeHg_2_T			g/m3	4.25E-06	4.25
C_Hg0_sed			g/m3	9.66E-06	9.66
C_HgII_1_sed			g/m3	7.91E+00	7,908,180.51
C_MeHg_1_sed			g/m3	1.23E-02	12,347.00
C_Hg0_sed, wet			g/g	3.65E-12	0.00
C_HgII_1_sed, wet			g/g	6.18E-06	6.18
C_MeHg_1_sed, wet			g/g	1.48E-08	0.01
C_HgT_sed,wet			g/g	6.19E-06	6.19
C_Hg0_sed, dry weight			g/g	2.14E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.76E-05	17.55
C_MeHg_1_sed, dry weight			g/g	2.74E-08	0.03
C_HgT_1			g/m3	4.32E-05	43.19
C_HgT_2			g/m3	3.08E-04	307.63
C_HgT_Sed, dry weight			g/g	1.76E-05	17.58
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.16%	82.24%	14.60%
Layer 2			1.38%	94.83%	3.78%
Sediments			0.16%	99.84%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.81571%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			2.94813%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61221%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			11.23203%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			3.93402%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			14.62272%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			17.42109%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			55.71087%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot A_w \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	6.303E-06	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	6.3E-06
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	3.552E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	3.6E-05
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T	1.366E-06	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	1.4E-06
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.164E-05	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	1.2E-05
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	2.917E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.00029
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T	4.252E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	4.3E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	9.662E-06	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	9.7E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	7.92E+00	C_HgII_1_sed	7.908E+00	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	7.90818
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed	1.235E-02	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.01235

A*x=b

Target C_sed, wet 7.920537175 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	134.70
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	122.63
kw_red_2	water column reduction rate constant	per yr	23.27
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for	per yr	0.82
kw_mer	water column *mer* cleavage demeth	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

$$kw_{v,i} = \frac{K_{v,1} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed} \cdot 3.1536x10^7}{z_{sed}}$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{C_{diss,i}^j + C_{DOC,i}^j} = \frac{TSS}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

		alphas		
	log K	layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.81571%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61221%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			2.94813%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93402%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			17.42109%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			14.62272%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.78562%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.16164%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00628%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.14683%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			73.17463%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.14319%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			73.80506%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			6.31498%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.99560%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.83
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	1.14
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	7,154.39
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot +K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed}+K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6}+K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	8.46	mg/L
Sbio_zoo,1	2.5		TSS_2	1.34	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	8.30E-01				
Sbio_dead,2	1.14E+00				
S_abio, sed	8.42E+04				
S_bio_dead,sed	7.15E+03				
S_sed,total	9.14E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

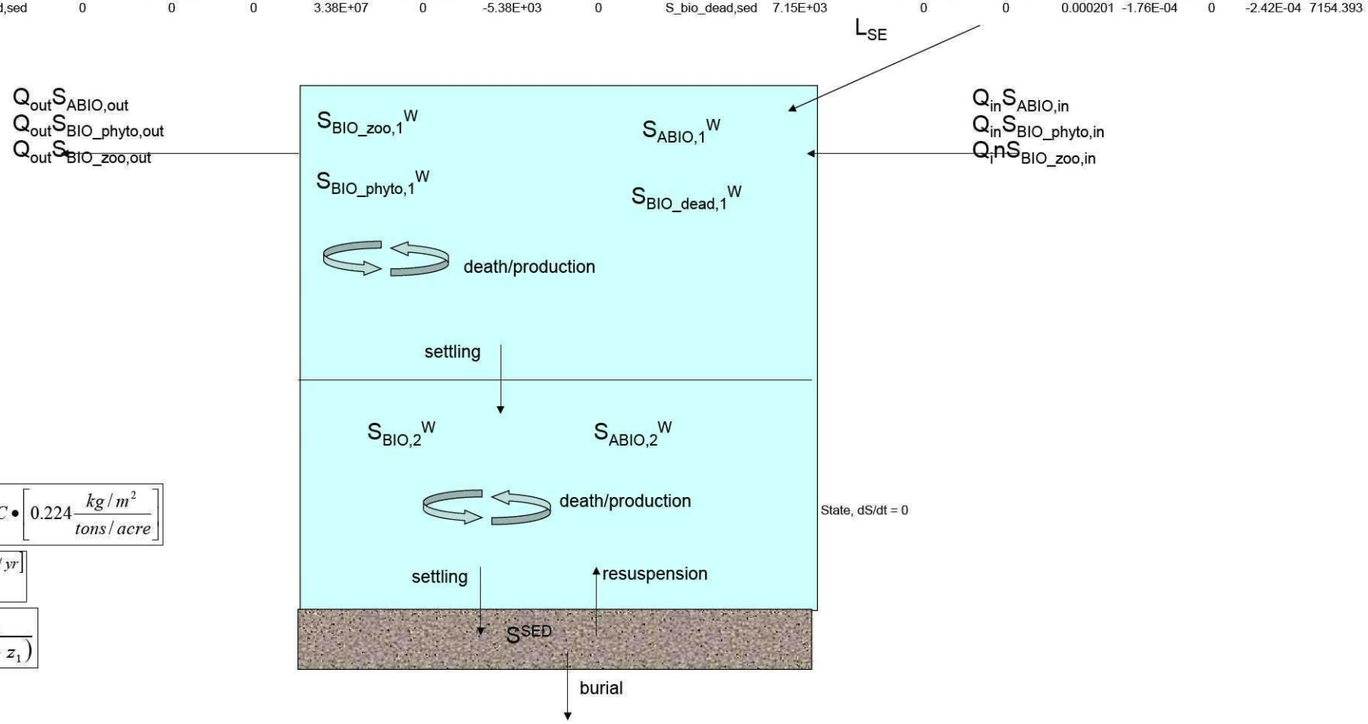
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	3.55E+07	S_bio_dead,1	8.30E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.829741
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	1.14E+00	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	1.138825
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	7.15E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	7154.393



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Belted Kingfisher – Varied Diet

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00816	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.03612		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03934		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.17421		
k_meth_1	abiotic methylation in layer 1		per yr	3.46E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	8.93E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.16E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.74E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.02E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	8.93E-06	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0	* currently assume no reduction in sediments	
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	1
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

$$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$$

1 UV-B is modeled as being 0.5% of visible light.
check?

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location		
East		YES
West		NO

Revisions		
Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Little Blue Heron

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury

Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Kd_abio		
HgII	7,182,936	1
MeHg	15,887	1
Kd_bio		
HgII	17,941,378	1
MeHg	2,581,565	1
Kd_DOC		
HgII	301,427	1
MeHg	310,000	1
	PCT ERROR	CLEANUP
MeHg Filtered	9.50	13.61
HgT Filtered	-51.71	
MeHg Unfilte	-64.28	
HgT Unfiltere	-46.85	

Inflow Mercury Concentrations

Hg0	0	g/m3			
HgII	5.64E-06	g/m3	5.64	-38.33653462	
MeHg	7.33E-08	g/m3	0.07332	43.08721129	Fish

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27	ug/g	

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	11.73	ng/L		-11.73	-100	0.47	ng/L	4.93	ng/L
	HgII Filtered	3.14	ng/L		-3.14	-100	0.13	ng/L	1.32	ng/L
Epilimnion	MeHg Filtered	0.43	ng/L	0.47525	0.04	9.5013533	0.03	ng/L	0.19	ng/L
	HgT Filtered	15.31	ng/L	7.39	-7.92	-51.71183	0.63	ng/L	6.44	ng/L
	Hg0 Unfiltered	11.73	ng/L		-11.73	-100	0.47	ng/L	4.93	ng/L
	HgII Unfiltered	66.10	ng/L		-66.10	-100	2.67	ng/L	27.78	ng/L
	MeHg Unfiltered	2.47	ng/L	0.88225	-1.59	-64.28243	0.18	ng/L	1.09	ng/L
	HgT Unfiltered	80.30	ng/L	42.67625	-37.62	-46.85323	3.32	ng/L	33.79	ng/L
Hypolimnion	Hg0 Filtered	21.98	ng/L		-21.98	-100	0.53	ng/L	9.02	ng/L
	HgII Filtered	116.08	ng/L		-116.08	-100	2.59	ng/L	47.51	ng/L
	MeHg Filtered	5.28	ng/L		-5.28	-100	0.23	ng/L	2.23	ng/L
	HgT Filtered	143.34	ng/L		-143.34	-100	3.36	ng/L	58.77	ng/L
	Hg0 Unfiltered	21.98	ng/L		-21.98	-100	0.53	ng/L	9.02	ng/L
	HgII Unfiltered	551.86	ng/L		-551.86	-100	12.34	ng/L	225.90	ng/L
	MeHg Unfiltered	7.89	ng/L		-7.89	-100	0.35	ng/L	3.33	ng/L
	HgT Unfiltered	581.74	ng/L		-581.74	-100	13.21	ng/L	238.26	ng/L
	Sediment									
	Hg0 porewater	21.98	ng/L		-21.98	-100	0.53	ng/L	9.024	ng/L
	HgII porewater	99.56	ng/L		-99.56	-100	2.18	ng/L	40.730	ng/L
	MeHg porewater	1.22	ng/L		-1.22	-100	0.05	ng/L	0.512	ng/L
	HgT porewater	122.77	ng/L		-122.77	-100	2.76	ng/L	50.266	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.22	ug/g		-33.22	-100	0.39	ug/g	13.59	ug/g
	MeHg bulk, dry	0.05107	ug/g	0.00422	-0.05	-91.73681	0.00	ug/g	0.02	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.730	ug/g	13.61	ug/g
	Trophic Level 3	0.40	ug/g		-0.40	-100	0.029	ug/g	0.17	ug/g
	Trophic Level 4	0.86	ug/g		-0.86	-100	0.063	ug/g	0.38	ug/g
	HI	2.27					0.17		1.00	
	Sensitive Indicator	Little Blue Heron					Little Blue Heron		Little Blue Heron	
	Target C_sed, dry	13.61	ug/g	Note: 8						
	Target C_sed, wet	6.13	ug/g							

Rate Constants

Process	Media	Value	Units		ratio Sed Meth/demeth
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		
1.00E-03	Sediment	3.49E-07	per day		
Demethylation	Epilimnion	1.16E-08	per day		
1.00E-03	Hypolimnion	1.16E-07	per day		50.00%
2.00E-03	Sediment	6.98E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

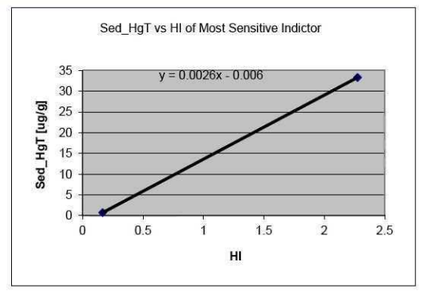
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.49	0.04	0.21
Otter	0.52	0.04	0.23
Mink	**1.02**	0.07	0.45
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	**2.27**	0.17	**1.00**
Pied-bill Grebe	0.93	0.07	0.41
Kingfisher	0.00	0.00	0.00
Wood Duck	0.36	0.03	0.16
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
2.27	33.27
0.17	0.73
m =	15.426
b=	-1.815
Sed_HgT	13.611
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

	Site-Specific User Input	Required
	Model Calculated	No input required
	Data Necessary for certain sites	Only necessary if applicable to site of interest
	Scenario 1 Output	
	Scenario 2 Output	
	Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.43	0.03	0.191	ng/L

Biota

Trophic Level 1: Phytoplankton	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Insects	0.07	0.01	0.03	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.03	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.40	0.03	0.17	ug Hg/ g wet weight
Trophic Level 4: Bass	0.86	0.06	0.38	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.47	0.03	0.21	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.08	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.03	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Body Weight	Ingestion Rate	Drinking rate	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants	Percent of Diet from Trophic Level 2 : Insects	Percent of Diet from Trophic Level 2 : Crayfish or Frogs	Percent of Diet from Trophic Level 3 : Fish	Percent of Diet from Trophic Level 4 : Fish	Percent of Diet from nonaquatic sources	Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Insects	Potential Dose from Trophic Level 2: Crayfish	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
Animal	[kg in wet weight]	[kg wet weight/d]	[L/d]	--	--	--	--	--	--	[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	36	0	0	0	36	75	0.49
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	29	9	39	75	0.52
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	70	76	75	**1.02**
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	25%	0%	75%	0%	0%	0	0	8	0	129	0	136	60	**2.27**
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	18	6	32	0	56	60	0.93
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	17	5	0	0	0	22	60	0.36
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	8	5000	0.00
Human	**Human Specific Parameters**																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Wildlife Specific Parameters | **Contaminated Sediment Calculations**

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.005	0.00	2.64	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.08	2.14	0.62	3	75	0.04
0.003	0.00	0.00	0.27	0.19	5.06	6	75	0.07
0.001	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.015	0.00	0.57	0.00	9.33	0.00	10	60	0.17
0.002	0.00	1.27	0.46	2.32	0.00	4	60	0.07
0.004	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.002	1.22	0.36	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.03	0.08	0.48	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.031	0.00	16.02	0.00	0.00	0.00	16	75	0.21
0.016	0.00	0.00	0.51	12.96	3.76	17	75	0.23
0.019	0.00	0.00	1.62	1.17	30.69	33	75	0.45
0.009	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.090	0.00	3.44	0.00	56.56	0.00	60	60	**1.00**
0.014	0.00	7.70	2.77	14.05	0.00	25	60	0.41
0.022	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.013	7.37	2.17	0.00	0.00	0.00	10	60	0.16
0.000	0.00	0.00	0.19	0.47	2.91	4	5000	0.00
							RfD	
0.003	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Little Blue Heron

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Little Blue Heron

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Coun	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeHg	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and reflec		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

this table does not all correspond to EPA Report to Congress - check!

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	
HgII	Mean	58,000	50000	100,000	200,000	
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000		
MeHg	Mean	7000	3000	100,000	500,000	
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000		
Hg0		1,000	1,000	3000	1,000	NTG added these 11/1/19

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893.2	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.38

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.71E-07	0.47
C_HgII_1_Aq			g/m3	1.27E-07	0.13
C_MeHg_1_Aq			g/m3	3.15E-08	0.03
C_Hg0_2_Aq			g/m3	5.32E-07	0.53
C_HgII_2_Aq			g/m3	2.59E-06	2.59
C_MeHg_2_Aq			g/m3	2.31E-07	0.23
C_Hg0_pore			g/m3	5.32E-07	0.53
C_HgII_pore			g/m3	2.18E-06	2.18
C_MeHg_pore			g/m3	4.76E-08	0.05
C_HgT_1_filtered			g/m3	6.30E-07	0.63
C_HgT_2_filtered			g/m3	3.36E-06	3.36
C_HgT_Sed_filtered			g/m3	2.76E-06	2.76
C_Hg0_1_T			g/m3	4.71E-07	0.47
C_HgII_1_T			g/m3	2.67E-06	2.67
C_MeHg_1_T			g/m3	1.79E-07	0.18
C_Hg0_2_T			g/m3	5.32E-07	0.53
C_HgII_2_T			g/m3	1.23E-05	12.34
C_MeHg_2_T			g/m3	3.45E-07	0.35
C_Hg0_sed, bulk			g/m3	4.42E-07	0
C_HgII_1_sed, bulk			g/m3	3.28E-01	328,097
C_MeHg_1_sed, bulk			g/m3	8.97E-04	897
C_Hg0_sed, wet			g/g	3.45E-13	0.000
C_HgII_1_sed, wet			g/g	3.93E-07	0.393
C_MeHg_1_sed, wet			g/g	6.65E-14	0.000
C_HgT_sed,wet			g/g	3.93E-07	0.393
C_Hg0_sed, dry weight			g/g	9.80E-13	0.0000
C_HgII_1_sed, dry weight			g/g	7.28E-07	0.7283
C_MeHg_1_sed, dry weight			g/g	1.99E-09	0.0020
C_HgT_1			g/m3	3.32E-06	3.321
C_HgT_2			g/m3	1.32E-05	13.213
C_HgT_Sed, dry weight			g/g	7.30E-07	0.730
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		5.40%	80.41%	14.19%
Layer 2			2.61%	93.36%	4.03%
Sediments			0.27%	99.73%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			1.000	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.008	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			0.029	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			1.000	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.036	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			0.112	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.000	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.039	
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			0.146	
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.000	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.174	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			0.557	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi}V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,A} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,A} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,A} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C Hg0 1 T	C HgII 1 T	C MeHg 1 T	C Hg0 2 T	C HgII 2 T	C MeHg 2 T	C Hg0 1 sed	C HgII 1 sed	C MeHg 1 sed
	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E+08	0.00E+00	0.00E+00	-5.25E+03	3.54E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03

A*x=b

Matrix b		Solution Matrix
-4.89E-01	C Hg0 1 T	4.712E-07
-6.18E+01	C HgII 1 T	2.670E-06
-1.43E+00	C MeHg 1 T	1.792E-07
0.00E+00	C Hg0 2 T	5.321E-07
0.00E+00	C HgII 2 T	1.234E-05
0.00E+00	C MeHg 2 T	3.452E-07
0.00E+00	C Hg0 sed	4.417E-07
0.00E+00	C HgII 1 sed	3.281E-01
0.00E+00	C MeHg 1 sed	8.968E-04

Inverted Matrix

-8.13E-09	-7.48E-09	-3.10E-09	-7.60E-09	-7.47E-09	-3.13E-09	-7.60E-09	-7.47E-09	-3.14E-09	4.71217E-07
-3.39E-08	-4.26E-08	-1.30E-08	-4.05E-08	-4.21E-08	-1.32E-08	-4.05E-08	-4.21E-08	-1.32E-08	2.67016E-06
-6.58E-10	-8.19E-10	-8.94E-08	-1.33E-09	-1.49E-09	-8.87E-08	-1.33E-09	-1.52E-09	-8.86E-08	1.79194E-07
-7.220E-09	-8.479E-09	-2.945E-09	-4.60E-08	-1.42E-08	-3.24E-09	-4.60E-08	-1.42E-08	-3.25E-09	5.3214E-07
-1.581E-07	-1.968E-07	-6.130E-08	-3.19E-07	-3.58E-07	-6.34E-08	-3.19E-07	-3.58E-07	-6.36E-08	1.23359E-05
-2.166E-09	-2.697E-09	-1.236E-07	-4.38E-09	-4.91E-09	-2.92E-07	-4.38E-09	-5.00E-09	-2.92E-07	3.45194E-07
-5.99E-09	-7.04E-09	-2.44E-09	-3.82E-08	-1.18E-08	-2.69E-09	-3.24E-06	-1.18E-08	-2.69E-09	4.41677E-07
-4.20E-03	-5.23E-03	-1.63E-03	-8.49E-03	-9.52E-03	-1.69E-03	-8.49E-03	-9.71E-03	-1.69E-03	0.328097232
-6.35E-06	-7.91E-06	-2.82E-04	-1.28E-05	-1.44E-05	-6.66E-04	-1.28E-05	-1.47E-05	-8.55E-04	0.000896776

x=b/A

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 1
Little Blue Heron

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.008
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.052
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.091
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.732
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.121
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.063
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.738
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.330
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		5.52E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		4.40E-05
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \quad \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.17E-05	11.73
C_HgII_1_Aq			g/m3	3.14E-06	3.14
C_MeHg_1_Aq			g/m3	4.34E-07	0.43
C_Hg0_2_Aq			g/m3	2.20E-05	21.98
C_HgII_2_Aq			g/m3	1.16E-04	116.08
C_MeHg_2_Aq			g/m3	5.28E-06	5.28
C_Hg0_pore			g/m3	2.20E-05	21.98
C_HgII_pore			g/m3	9.96E-05	99.56
C_MeHg_pore			g/m3	1.22E-06	1.22
C_HgT_1_filtered			g/m3	1.53E-05	15.31
C_HgT_2_filtered			g/m3	1.43E-04	143.34
C_HgT_Sed_filtered			g/m3	1.23E-04	122.77
C_Hg0_1_T			g/m3	1.17E-05	11.73
C_HgII_1_T			g/m3	6.61E-05	66.10
C_MeHg_1_T			g/m3	2.47E-06	2.47
C_Hg0_2_T			g/m3	2.20E-05	21.98
C_HgII_2_T			g/m3	5.52E-04	551.86
C_MeHg_2_T			g/m3	7.89E-06	7.89
C_Hg0_sed			g/m3	1.82E-05	18.25
C_HgII_1_sed			g/m3	1.50E+01	14965109.78
C_MeHg_1_sed			g/m3	2.30E-02	23006.97
C_Hg0_sed, wet			g/g	6.89E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.687
C_MeHg_1_sed, wet			g/g	2.75E-08	0.028
C_HgT_sed,wet			g/g	1.17E-05	11.714
C_Hg0_sed, dry weight			g/g	4.05E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.32E-05	33.22
C_MeHg_1_sed, dry weight			g/g	5.11E-08	0.05
C_HgT_1			g/m3	8.03E-05	80.30
C_HgT_2			g/m3	5.82E-04	581.74
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.08%	82.31%	14.61%
Layer 2			1.36%	94.86%	3.78%
Sediments			0.15%	99.85%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.81571%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	2.94813%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	3.61221%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.93402%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	14.62272%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	17.42109%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03550%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{metR} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{metR} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{metR} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{metR2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2) from Mortimer, cited in Schnoor, 1996, pg. 57. for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix											x=b/A
1.173E-05	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	1.17E-05	C_Hg0_1_T	
6.610E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	6.61E-05	C_HgII_1_T	
2.470E-06	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	2.47E-06	C_MeHg_1_T	
2.198E-05	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	2.2E-05	C_Hg0_2_T	
5.519E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.000552	C_HgII_2_T	
7.888E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	7.89E-06	C_MeHg_2_T	
1.825E-05	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	1.82E-05	C_Hg0_sed	
1.497E+01	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	14.96511	C_HgII_1_sed	
2.301E-02	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.023007	C_MeHg_1_sed	

A*x=b

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}\left(1-\theta_{sed}\right)} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

C_T_sed 14.988135 g/m3

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	13900.95
TSS_1			mg/L	8.46
TSS+2			mg/L	1.34
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_Hg0_1	Effective K for Hg0 in layer 2		L/kg	2.37E+06
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.54E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	3.69E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.93E-06	4.93
C_HgII_1_Aq			g/m3	1.32E-06	1.32
C_MeHg_1_Aq			g/m3	1.91E-07	0.19
C_Hg0_2_Aq			g/m3	9.02E-06	9.02
C_HgII_2_Aq			g/m3	4.75E-05	47.51
C_MeHg_2_Aq			g/m3	2.23E-06	2.23
C_Hg0_pore			g/m3	9.02E-06	9.02
C_HgII_pore			g/m3	4.07E-05	40.73
C_MeHg_pore			g/m3	5.12E-07	0.51
C_HgT_1_filtered			g/m3	6.44E-06	6.44
C_HgT_2_filtered			g/m3	5.88E-05	58.77
C_HgT_Sed_filtered			g/m3	5.03E-05	50.27
C_Hg0_1_T			g/m3	4.93E-06	4.93
C_HgII_1_T			g/m3	2.78E-05	27.78
C_MeHg_1_T			g/m3	1.09E-06	1.09
C_Hg0_2_T			g/m3	9.02E-06	9.02
C_HgII_2_T			g/m3	2.26E-04	225.90
C_MeHg_2_T			g/m3	3.33E-06	3.33
C_Hg0_sed			g/m3	7.49E-06	7.49
C_HgII_1_sed			g/m3	6.12E+00	6,122,004.99
C_MeHg_1_sed			g/m3	9.65E-03	9,648.86
C_Hg0_sed, wet			g/g	2.83E-12	0.00
C_HgII_1_sed, wet			g/g	4.78E-06	4.78
C_MeHg_1_sed, wet			g/g	1.16E-08	0.01
C_HgT_sed,wet			g/g	4.79E-06	4.79
C_Hg0_sed, dry weight			g/g	1.66E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.36E-05	13.59
C_MeHg_1_sed, dry weight			g/g	2.14E-08	0.02
C_HgT_1			g/m3	3.38E-05	33.79
C_HgT_2			g/m3	2.38E-04	238.26
C_HgT_Sed, dry weight			g/g	1.36E-05	13.61
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.21%	82.20%	14.59%
Layer 2			1.40%	94.81%	3.79%
Sediments			0.16%	99.84%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.81571%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	2.94813%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	3.61221%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.93402%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	14.62272%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	17.42109%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	55.71087%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{Hg1,1} + \left[kw_{mer} \cdot V_w + kw_{photored,1} \cdot V_w\right] \cdot C^w_{MeHg,1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{s,2} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg,1} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red,1} \cdot V_w - kw_{meth,1} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abiaHgII} A_w - v_{s,2} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg,1}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth,1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth,1} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s,1} \cdot f^{w,1}_{abiaMeHg} A_w - v_{s,2} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg,1} + Q' \cdot C^w_{MeHg,2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photored,2} V_w\right] \cdot C^w_{MeHg,2} + \left[-Q' - kw_{oxid} V_w - v_{s,1} \cdot f^{w,2}_{abiaHg0} \cdot A_w - v_{s,2} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg,2} + \left[-Q' - kw_{red,2} \cdot V_w - kw_{meth,2} \cdot V_w - v_{s,1} \cdot f^{w,2}_{abiaHgII} A_w - v_{s,2} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg,2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{s,1} \cdot f^{w,2}_{abiaMeHg} A_w - v_{s,2} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg,2} + Q' \cdot C^w_{MeHg,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{s,1} \cdot f^{w,2}_{abiaHg0} + v_{s,2} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{s,1} \cdot f^{w,2}_{abiaHgII} + v_{s,2} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{s,1} \cdot f^{w,2}_{abiaMeHg} + v_{s,2} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	6.13E+00	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed

A*x=b

Target C_sed, wet 6.131661347 g/g

Solution Matrix	Inverted Matrix										x=b/A
4.929E-06	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	4.93E-06	
2.778E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	2.78E-05	
1.086E-06	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	1.09E-06	
9.024E-06	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	9.02E-06	
2.259E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.000226	
3.331E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	3.33E-06	
7.490E-06	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	7.49E-06	
6.122E+00	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	6.122005	
9.649E-03	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.009649	

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate cc	per yr	134.70
kw_v,HgII	water column volatilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatilization loss rate cc	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	122.63
kw_red_2	water column reduction rate constant,	per yr	23.27
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for I	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for I	per yr	0.82
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \Big/ \frac{C_{diss,i}^j + C_{DOC,i}^j}{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)} = \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} \Big/ C_{filtered,i}^j$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.81571%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61221%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			2.94813%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			11.23203%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93402%	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			17.42109%	
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			14.62272%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			55.71087%	
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%	
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%	
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.78562%	
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.16164%	
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00628%	
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03550%	
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%	
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%	
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.14683%	
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%	
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%	
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%	
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%	
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%	
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			73.17463%	
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%	
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%	
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%	
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%	
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%	
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.14319%	
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			73.80506%	
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			6.31498%	
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			33.02160%	
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%	
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00055%	
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.00440%	
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%	
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99945%	
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.99560%	
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5	from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5	
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0	
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0	
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13	
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20	
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.83	
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	1.14	
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58	
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	7,154.39	

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

DOC_1	Dissolved Organic Carbon Concentration in Layer 1	g/m3	16	
DOC_2	Dissolved Organic Carbon Concentration in Layer 2	g/m3	16	
Symbol	**Parameter**	**Units**	**Value**	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	8.46	mg/L
Sbio_zoo,1	2.5		TSS_2	1.34	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	8.30E-01				
Sbio_dead,2	1.14E+00				
S_abio, sed	8.42E+04				
S_bio_dead,sed	7.15E+03				
S_sed,total	9.14E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

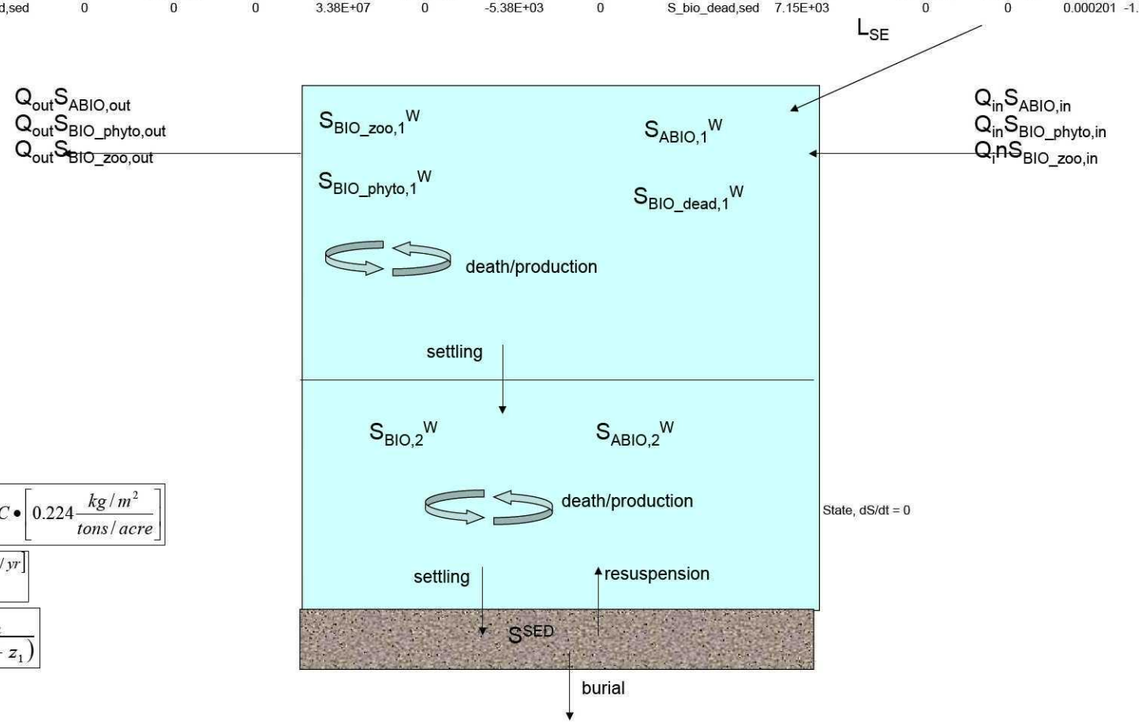
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	3.55E+07	S_bio_dead,1	8.30E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.829741
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	1.14E+00	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	1.138825
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	7.15E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	7154.393



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00816	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.03612		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03934		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.17421		
k_meth_1	abiotic methylation in layer 1		per yr	3.46E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	8.93E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.16E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.74E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.02E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	8.93E-06	

$$k_{demeth} = k_{demeth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that
only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation
suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability.
Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s

2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

1 UV-B is modeled as being 0.5% of visible light.
check?

1

$$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV-B} = 0.4415 * (DOC)^{.86}$$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43* ,135.

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 1 – Mink

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	463,365	m2	
Epilimnion Depth	1.4	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	6.80E+06		
Outflow	6.80E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	152.4	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	-38.33653462
MeHg	7.33E-08	g/m3	0.07332	43.08721129

Total Mercury Concentration in Contaminated Sediment, dry weight	33.27	ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio

HgII	7,182,936	1
MeHg	15,887	1

Kd_bio

HgII	17,941,378	1
MeHg	2,581,565	1

Kd_DOC

HgII	301,427	1
MeHg	310,000	1

	PCT ERROR	CLEANUP
MeHg Filtered	9.50	32.74
HgT Filtered	-51.71	
MeHg Unfilter	-64.28	
HgT Unfiltere	-46.85	

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	11.73	ng/L		-11.73	-100	0.47	ng/L	11.55	ng/L
	HgII Filtered	3.14	ng/L		-3.14	-100	0.13	ng/L	3.09	ng/L
Epilimnion	MeHg Filtered	0.43	ng/L	0.47525	0.04	9.5013533	0.03	ng/L	0.43	ng/L
	HgT Filtered	15.31	ng/L	7.39	-7.92	-51.71183	0.63	ng/L	15.07	ng/L
	Hg0 Unfiltered	11.73	ng/L		-11.73	-100	0.47	ng/L	11.55	ng/L
	HgII Unfiltered	66.10	ng/L		-66.10	-100	2.67	ng/L	65.05	ng/L
	MeHg Unfiltered	2.47	ng/L	0.88225	-1.59	-64.28243	0.18	ng/L	2.43	ng/L
	HgT Unfiltered	80.30	ng/L	42.67625	-37.62	-46.85323	3.32	ng/L	79.03	ng/L
Hypolimnion	Hg0 Filtered	21.98	ng/L		-21.98	-100	0.53	ng/L	21.63	ng/L
	HgII Filtered	116.08	ng/L		-116.08	-100	2.59	ng/L	114.21	ng/L
	MeHg Filtered	5.28	ng/L		-5.28	-100	0.23	ng/L	5.20	ng/L
	HgT Filtered	143.34	ng/L		-143.34	-100	3.36	ng/L	141.04	ng/L
	Hg0 Unfiltered	21.98	ng/L		-21.98	-100	0.53	ng/L	21.63	ng/L
	HgII Unfiltered	551.86	ng/L		-551.86	-100	12.34	ng/L	542.99	ng/L
	MeHg Unfiltered	7.89	ng/L		-7.89	-100	0.35	ng/L	7.76	ng/L
	HgT Unfiltered	581.74	ng/L		-581.74	-100	13.21	ng/L	572.39	ng/L
	Sediment									
	Hg0 porewater	21.98	ng/L		-21.98	-100	0.53	ng/L	21.631	ng/L
	HgII porewater	99.56	ng/L		-99.56	-100	2.18	ng/L	97.963	ng/L
	MeHg porewater	1.22	ng/L		-1.22	-100	0.05	ng/L	1.201	ng/L
	HgT porewater	122.77	ng/L		-122.77	-100	2.76	ng/L	120.796	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	33.22	ug/g		-33.22	-100	0.39	ug/g	32.68	ug/g
	MeHg bulk, dry	0.05107	ug/g	0.00422	-0.05	-91.73681	0.00	ug/g	0.05	ug/g
	HgT bulk, dry	33.27	ug/g	33.27	0.00	0	0.730	ug/g	32.74	ug/g
Fish	Trophic Level 3	0.40	ug/g		-0.40	-100	0.029	ug/g	0.39	ug/g
	Trophic Level 4	0.86	ug/g		-0.86	-100	0.063	ug/g	0.85	ug/g
	HI	1.02					0.07		1.00	
	Sensitive Indicator	Mink					Mink		Mink	
	Target C_sed, dry	32.74	ug/g	Note: 8						
	Target C_sed, wet	14.75	ug/g							

Rate Constants

Process	Media	Value	Units		
Methylation	Epilimnion	1.16E-07	per day	1.16E-04	
	Hypolimnion	1.16E-06	per day		ratio Sed
1.00E-03	Sediment	3.49E-07	per day		Meth/demeth
Demethylation	Epilimnion	1.16E-08	per day		50.00%
1.00E-03	Hypolimnion	1.16E-07	per day		
2.00E-03	Sediment	6.98E-07	per day		
Biotic Reduction	Water Column	0.03	per day		
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day		
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day		
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day		
Dark Oxidation	Water Column	1.44	per day		

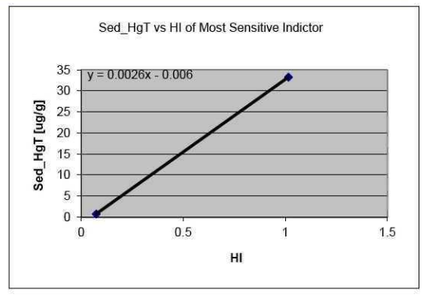
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.49	0.04	0.48
Otter	0.52	0.04	0.51
Mink	**1.02**	0.07	1.00
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	0.93	0.07	0.92
Kingfisher	0.00	0.00	0.00
Wood Duck	0.36	0.03	0.36
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
1.02	33.27
0.07	0.73
m =	34.550
b=	-1.815
Sed_HgT	32.735
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.43	0.03	0.427	ng/L

Biota

Trophic Level 1: Phytoplankton	0.08	0.01	0.08	ug Hg/ g wet weight
Trophic Level 2: Insects	0.07	0.01	0.07	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.08	0.01	0.08	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.40	0.03	0.39	ug Hg/ g wet weight
Trophic Level 4: Bass	0.86	0.06	0.85	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.47	0.03	0.46	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.08	0.01	0.08	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.08	0.01	0.07	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Wildlife Specific Parameters									Contaminated Sediment Calculations								
Animal	Body Weight [kg in wet weight]	Ingestion Rate [kg wet weight/d]	Drinking rate [L/d]	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants --	Percent of Diet from Trophic Level 2 : Insects --	Percent of Diet from Trophic Level 2 : Crayfish or Frogs --	Percent of Diet from Trophic Level 3 : Fish --	Percent of Diet from Trophic Level 4 : Fish --	Percent of Diet from nonaquatic sources --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	36	0	0	0	36	75	0.49
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	1	29	9	39	75	0.52
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	4	3	70	76	75	**1.02**
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	18	6	32	0	56	60	0.93
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	17	5	0	0	0	22	60	0.36
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	0	1	7	8	5000	0.00
Human	**Human Specific Parameters**																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.005	0.00	2.64	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.08	2.14	0.62	3	75	0.04
0.003	0.00	0.00	0.27	0.19	5.06	6	75	0.07
0.001	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.015	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.002	0.00	1.27	0.46	2.32	0.00	4	60	0.07
0.004	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.002	1.22	0.36	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.03	0.08	0.48	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.068	0.00	35.88	0.00	0.00	0.00	36	75	0.48
0.036	0.00	0.00	1.14	29.02	8.42	39	75	0.51
0.043	0.00	0.00	3.63	2.63	68.74	75	75	1.00
0.019	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.201	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.031	0.00	17.25	6.20	31.48	0.00	55	60	0.92
0.048	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.029	16.51	4.86	0.00	0.00	0.00	21	60	0.36
0.000	0.00	0.00	0.43	1.06	6.52	8	5000	0.00
							RfD	
0.008	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	4.63E+05	Link
z_1	Thickness of Layer 1		m	1.40E+00	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	6.49E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	4.63E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	6.80E+06	Calc
Qout	Outflow		m3/yr	6.80E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	152.4	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.71E-07	0.47
C_HgII_1_Aq			g/m3	1.27E-07	0.13
C_MeHg_1_Aq			g/m3	3.15E-08	0.03
C_Hg0_2_Aq			g/m3	5.32E-07	0.53
C_HgII_2_Aq			g/m3	2.59E-06	2.59
C_MeHg_2_Aq			g/m3	2.31E-07	0.23
C_Hg0_pore			g/m3	5.32E-07	0.53
C_HgII_pore			g/m3	2.18E-06	2.18
C_MeHg_pore			g/m3	4.76E-08	0.05
C_HgT_1_filtered			g/m3	6.30E-07	0.63
C_HgT_2_filtered			g/m3	3.36E-06	3.36
C_HgT_Sed_filtered			g/m3	2.76E-06	2.76
C_Hg0_1_T			g/m3	4.71E-07	0.47
C_HgII_1_T			g/m3	2.67E-06	2.67
C_MeHg_1_T			g/m3	1.79E-07	0.18
C_Hg0_2_T			g/m3	5.32E-07	0.53
C_HgII_2_T			g/m3	1.23E-05	12.34
C_MeHg_2_T			g/m3	3.45E-07	0.35
C_Hg0_sed, bulk			g/m3	4.42E-07	0
C_HgII_1_sed, bulk			g/m3	3.28E-01	328,097
C_MeHg_1_sed, bulk			g/m3	8.97E-04	897
C_Hg0_sed, wet			g/g	3.45E-13	0.000
C_HgII_1_sed, wet			g/g	3.93E-07	0.393
C_MeHg_1_sed, wet			g/g	6.65E-14	0.000
C_HgT_sed,wet			g/g	3.93E-07	0.393
C_Hg0_sed, dry weight			g/g	9.80E-13	0.0000
C_HgII_1_sed, dry weight			g/g	7.28E-07	0.7283
C_MeHg_1_sed, dry weight			g/g	1.99E-09	0.0020
C_HgT_1			g/m3	3.32E-06	3.321
C_HgT_2			g/m3	1.32E-05	13.213
C_HgT_Sed, dry weight			g/g	7.30E-07	0.730

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)	5.40%	80.41%	14.19%
Layer 2		2.61%	93.36%	4.03%
Sediments		0.27%	99.73%	0.00%

Q'	Bulk Exchange Flow		m3/yr	5,858,941
Qin	Inflow		m3/yr	6,796,715
Qout	Outflow		m3/yr	6,796,715
Aw	Surface Area of the Water Body		m2	463,365
E	Exchange rate		m2/yr	9
V_1	Volume of Layer 1	Aw*z_1	m3	648,711
V_2	Volume of Layer 2	Aw*z_2	m3	46,337
z1	depth of first water layer		m	1.40
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.008
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.029
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.036
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.112
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.039
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.146
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.174
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.557

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi}V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abiHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,Hg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,MeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C Hg0 1 T	C HgII 1 T	C MeHg 1 T	C Hg0 2 T	C HgII 2 T	C MeHg 2 T	C Hg0 1 sed	C HgII 1 sed	C MeHg 1 sed
	1	2	3	4	5	6	7	8	9
C Hg0 1 T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C HgII 1 T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C MeHg 1 T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00
C Hg0 2 T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E+08	0.00E+00	0.00E+00	-5.25E+03	3.54E+00
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03

A*x=b

Matrix b	
C Hg0 1 T	4.712E-07
C HgII 1 T	2.670E-06
C MeHg 1 T	1.792E-07
C Hg0 2 T	5.321E-07
C HgII 2 T	1.234E-05
C MeHg 2 T	3.452E-07
C Hg0 sed	4.417E-07
C HgII 1 sed	3.281E-01
C MeHg 1 sed	8.968E-04

Solution Matrix	Inverted Matrix									x=b/A
-4.89E-01	-8.13E-09	-7.48E-09	-3.10E-09	-7.60E-09	-7.47E-09	-3.12E-09	-7.60E-09	-7.47E-09	-3.14E-09	4.71217E-07
-6.18E+01	-3.39E-08	-4.26E-08	-1.30E-08	-4.05E-08	-4.21E-08	-1.32E-08	-4.05E-08	-4.21E-08	-1.32E-08	2.67016E-06
-1.43E+00	-6.58E-10	-8.19E-10	-8.94E-08	-1.33E-09	-1.49E-09	-8.87E-08	-1.33E-09	-1.52E-09	-8.86E-08	1.79194E-07
0.00E+00	-7.220E-09	-8.479E-09	-2.945E-09	-4.60E-08	-1.42E-08	-3.24E-09	-4.60E-08	-1.42E-08	-3.25E-09	5.3214E-07
0.00E+00	-1.581E-07	-1.968E-07	-6.130E-08	-3.19E-07	-3.58E-07	-6.34E-08	-3.19E-07	-3.58E-07	-6.36E-08	1.23359E-05
0.00E+00	-2.166E-09	-2.697E-09	-1.236E-07	-4.38E-09	-4.91E-09	-2.92E-07	-4.38E-09	-5.00E-09	-2.92E-07	3.45194E-07
0.00E+00	-5.99E-09	-7.04E-09	-2.44E-09	-3.82E-08	-1.18E-08	-2.69E-09	-3.24E-06	-1.18E-08	-2.69E-09	4.41677E-07
0.00E+00	-4.20E-03	-5.23E-03	-1.63E-03	-8.49E-03	-9.52E-03	-1.69E-03	-8.49E-03	-9.71E-03	-1.69E-03	0.328097232
0.00E+00	-6.35E-06	-7.91E-06	-2.82E-04	-1.28E-05	-1.44E-05	-6.66E-04	-1.28E-05	-1.47E-05	-8.55E-04	0.000896776

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.008
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.052
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.091
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.732
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.381
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.121
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.063
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.738
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.330
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		5.52E-06
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		4.40E-05
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org,i}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}} \quad \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.17E-05	11.73
C_HgII_1_Aq			g/m3	3.14E-06	3.14
C_MeHg_1_Aq			g/m3	4.34E-07	0.43
C_Hg0_2_Aq			g/m3	2.20E-05	21.98
C_HgII_2_Aq			g/m3	1.16E-04	116.08
C_MeHg_2_Aq			g/m3	5.28E-06	5.28
C_Hg0_pore			g/m3	2.20E-05	21.98
C_HgII_pore			g/m3	9.96E-05	99.56
C_MeHg_pore			g/m3	1.22E-06	1.22
C_HgT_1_filtered			g/m3	1.53E-05	15.31
C_HgT_2_filtered			g/m3	1.43E-04	143.34
C_HgT_Sed_filtered			g/m3	1.23E-04	122.77
C_Hg0_1_T			g/m3	1.17E-05	11.73
C_HgII_1_T			g/m3	6.61E-05	66.10
C_MeHg_1_T			g/m3	2.47E-06	2.47
C_Hg0_2_T			g/m3	2.20E-05	21.98
C_HgII_2_T			g/m3	5.52E-04	551.86
C_MeHg_2_T			g/m3	7.89E-06	7.89
C_Hg0_sed			g/m3	1.82E-05	18.25
C_HgII_1_sed			g/m3	1.50E+01	14965109.78
C_MeHg_1_sed			g/m3	2.30E-02	23006.97
C_Hg0_sed, wet			g/g	6.89E-12	0.000
C_HgII_1_sed, wet			g/g	1.17E-05	11.687
C_MeHg_1_sed, wet			g/g	2.75E-08	0.028
C_HgT_sed,wet			g/g	1.17E-05	11.714
C_Hg0_sed, dry weight			g/g	4.05E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.32E-05	33.22
C_MeHg_1_sed, dry weight			g/g	5.11E-08	0.05
C_HgT_1			g/m3	8.03E-05	80.30
C_HgT_2			g/m3	5.82E-04	581.74
C_HgT_Sed			g/g	3.33E-05	33.27
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.08%	82.31%	14.61%
Layer 2			1.36%	94.86%	3.78%
Sediments			0.15%	99.85%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1.40	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.81571%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	2.94813%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	3.61221%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	3.93402%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	14.62272%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	17.42109%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.03550%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{vol Hg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{vol HgII} V_w - kw_{red1} \cdot V_w - kw_{metR} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg1}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{metB} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q_{out} - Q' - kw_{vol MeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg1} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg1} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg1} + \left[-Q' - kw_{red2} \cdot V_w - kw_{metR} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{metB2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2} + Q' \cdot C^w_{MeHg1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w}{\theta_{sed}}\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.50E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix											x=b/A
1.173E-05	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	1.17E-05	C_Hg0_1_T	
6.610E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	6.61E-05	C_HgII_1_T	
2.470E-06	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	2.47E-06	C_MeHg_1_T	
2.198E-05	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	2.2E-05	C_Hg0_2_T	
5.519E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.000552	C_HgII_2_T	
7.888E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	7.89E-06	C_MeHg_2_T	
1.825E-05	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	1.82E-05	C_Hg0_sed	
1.497E+01	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	14.96511	C_HgII_1_sed	
2.301E-02	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.023007	C_MeHg_1_sed	

A*x=b

C_T_sed 14.988135 g/m3

$$C^{sed}_{dry.}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	orgaanic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	orgaanic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	orgaanic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	orgaanic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	134.70
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	122.63
kw_red_2	water column reduction rate constant, layer 2	per yr	23.27
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	0.82
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity		m/yr		4792.628412
v_sB	biotic settling velocity		m/yr		73
v_rs	resuspension velocity		m/yr		0.003700005
k_mort	phytoplankton mortality rate		per yr		10.95
v_min	mineralization rate		per yr		0.01
v_bur	burial rate		m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0			m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII			m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg			m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0			m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII			m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg			m2/sec	6.11E-10
rho_s	Sediment Particle Density			g/cm3	2.65E+00
θ_sed	sediment porosity			cm3/cm3	0.83
z_sed	sediment layer,char mixing length			m	0.03
V_sed	Volume of Sediment	Aw*z_sed		m3	13900.95
TSS_1				mg/L	8.46
TSS+2				mg/L	1.34
Effective Partition Coefficients for each Hg species and layer					
K_eff_Hg0_1	Effective K for Hg0 in layer 1			L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2			L/kg	2.37E+06
K_eff_MeHg_1	Effective K for HgII in layer 1			L/kg	5.54E+05
K_eff_Hg0_2	Effective K for HgII in layer 2			L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1			L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2			L/kg	3.69E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.15E-05	11.55
C_HgII_1_Aq			g/m3	3.09E-06	3.09
C_MeHg_1_Aq			g/m3	4.27E-07	0.43
C_Hg0_2_Aq			g/m3	2.16E-05	21.63
C_HgII_2_Aq			g/m3	1.14E-04	114.21
C_MeHg_2_Aq			g/m3	5.20E-06	5.20
C_Hg0_pore			g/m3	2.16E-05	21.63
C_HgII_pore			g/m3	9.80E-05	97.96
C_MeHg_pore			g/m3	1.20E-06	1.20
C_HgT_1_filtered			g/m3	1.51E-05	15.07
C_HgT_2_filtered			g/m3	1.41E-04	141.04
C_HgT_Sed_filtered			g/m3	1.21E-04	120.80
C_Hg0_1_T			g/m3	1.15E-05	11.55
C_HgII_1_T			g/m3	6.51E-05	65.05
C_MeHg_1_T			g/m3	2.43E-06	2.43
C_Hg0_2_T			g/m3	2.16E-05	21.63
C_HgII_2_T			g/m3	5.43E-04	542.99
C_MeHg_2_T			g/m3	7.76E-06	7.76
C_Hg0_sed			g/m3	1.80E-05	17.95
C_HgII_1_sed			g/m3	1.47E+01	14,724,485.94
C_MeHg_1_sed			g/m3	2.26E-02	22,643.49
C_Hg0_sed, wet			g/g	6.78E-12	0.00
C_HgII_1_sed, wet			g/g	1.15E-05	11.50
C_MeHg_1_sed, wet			g/g	2.71E-08	0.03
C_HgT_sed,wet			g/g	1.15E-05	11.53
C_Hg0_sed, dry weight			g/g	3.99E-11	0.00
C_HgII_1_sed, dry weight			g/g	3.27E-05	32.68
C_MeHg_1_sed, dry weight			g/g	5.03E-08	0.05
C_HgT_1			g/m3	7.90E-05	79.03
C_HgT_2			g/m3	5.72E-04	572.39
C_HgT_Sed, dry weight			g/g	3.27E-05	32.74
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		3.08%	82.31%	14.61%
Layer 2			1.36%	94.86%	3.78%
Sediments			0.15%	99.85%	0.00%
Q'	Bulk Exchange Flow		m3/yr	5,858,941	
Qin	Inflow		m3/yr	6,796,715	
Qout	Outflow		m3/yr	6,796,715	
Aw	Surface Area of the Water Body		m2	463,365	
E	Exchange rate		m2/yr	9	
V_1	Volume of Layer 1	Aw*z_1	m3	648,711	
V_2	Volume of Layer 2	Aw*z_2	m3	46,337	
z1	depth of first water layer		m	1	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.81571%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			2.94813%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61221%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			11.23203%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			3.93402%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			14.62272%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			17.42109%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			55.71087%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{med2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-4.60E+08	7.96E+07	4.22E+06	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.89E-01	C_Hg0_1_T	1.155E-05	-4.89E-09	-3.46E-09	-1.63E-09	-1.07E-09	-1.46E-10	-1.33E-09	-1.06E-09	7.68E-07	-1.18E-09	1.2E-05
C_HgII_1_T	3.60E+08	-1.14E+08	1.31E-01	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-6.18E+01	C_HgII_1_T	6.505E-05	-1.56E-08	-1.99E-08	-4.69E-09	-3.70E-09	-8.24E-10	-3.01E-09	-3.68E-09	4.33E-06	-2.18E-09	6.5E-05
C_MeHg_1_T	0.00E+00	2.25E-01	-1.93E+07	0.00E+00	0.00E+00	5.86E+06	0.00E+00	0.00E+00	0.00E+00	-1.43E+00	C_MeHg_1_T	2.432E-06	-2.89E-16	-4.35E-16	-8.91E-08	4.05E-15	-2.37E-16	-8.83E-08	5.04E-13	1.56E-07	-8.82E-08	2.4E-06
C_Hg0_2_T	5.859E+06	0.000E+00	0.000E+00	-3.05E+07	1.08E+06	3.81E+04	3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	2.163E-05	-1.059E-09	-8.080E-10	-1.459E-10	-3.35E-08	-2.79E-10	2.04E-10	-3.35E-08	1.46E-06	4.82E-10	2.2E-05
C_HgII_2_T	0.000E+00	2.741E+07	0.000E+00	2.44E+07	-1.47E+08	4.14E-01	0.00E+00	5.25E+03	0.00E+00	0.00E+00	C_HgII_2_T	5.430E-04	-3.102E-09	-3.862E-09	9.097E-09	-6.26E-09	-7.02E-09	2.32E-08	-6.15E-09	3.68E-05	3.02E-08	0.00054
C_MeHg_2_T	0.000E+00	0.000E+00	8.134E+06	0.00E+00	4.14E-01	-1.79E+07	0.00E+00	0.00E+00	5.26E+03	0.00E+00	C_MeHg_2_T	7.764E-06	-3.520E-16	-6.689E-16	-1.226E-07	1.35E-14	-7.49E-16	-2.91E-07	1.66E-12	5.15E-07	-2.91E-07	7.8E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.59E+05	0.00E+00	0.00E+00	-3.12E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	1.795E-05	-8.79E-10	-6.71E-10	-1.21E-10	-2.78E-08	-2.32E-10	1.69E-10	-3.23E-06	1.21E-06	4.00E-10	1.8E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.47E+01	C_HgII_1_sed	1.472E+01	8.80E-10	6.72E-10	2.79E-04	2.78E-08	2.33E-10	6.62E-04	3.23E-06	9.98E-01	8.52E-04	14.7245
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E+07	0.00E+00	1.77E+00	-5.26E+03	0.00E+00	C_MeHg_1_sed	2.264E-02	-5.06E-13	-1.30E-12	-2.79E-04	4.00E-11	-1.63E-12	-6.62E-04	4.87E-09	1.51E-03	-8.52E-04	0.02264

A*x=b

Target C_sed, wet 14.74714739 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.78562%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00628%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		5.16164%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.14683%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		73.17463%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		38.05394%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		12.14319%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		6.31498%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		73.80506%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.99560%
L_T,Hg0	Total Load, Hg0	g/yr	4.89E-01
L_T,HgII	Total Load, HgII	g/yr	2.35E+01
L_T,MeHg	Total Load, MeHg	g/yr	9.36E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	134.70
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.22
kw_oxid_1	water column oxidation rate constant	per yr	554.95
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	122.63
kw_red_2	water column reduction rate constant	per yr	23.27
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	6.51
kw_photodegrad_2	water column photoreduction rate for	per yr	0.82
kw_mer	water column *mer* cleavage demeth	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.59E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.59E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.47E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	13900.95
TSS_1		mg/L	8.46
TSS+2		mg/L	1.34
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.37E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.54E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.81E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.69E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{}{C_{diss,i}^j + C_{DOC,i}^j} \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.49
L_T,HgII	Total Load, HgII		g/yr	23.51
L_T,MeHg	Total Load, MeHg		g/yr	0.94

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**8.96**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.175429989**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3786

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.2286	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	152.4	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.64**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.07**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.75**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.49**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.82**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	4.89E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	8.24E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	7.53E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	4.63E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = \left(1.32 + 0.009 \bullet T_a\right)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.81571%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61221%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			2.94813%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			11.23203%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93402%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			17.42109%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			14.62272%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			55.71087%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.78562%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			5.16164%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00628%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.03550%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.14683%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			73.17463%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			38.05394%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			12.14319%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			73.80506%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			6.31498%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			33.02160%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00055%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.00440%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99945%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.99560%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.13
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.20
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.83
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	1.14
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	84,224.58
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	7,154.39
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	8.46	mg/L
Sbio_zoo,1	2.5		TSS_2	1.34	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	1.34E-01				
Sabio_2	1.99E-01				
Sbio_dead,1	8.30E-01				
Sbio_dead,2	1.14E+00				
S_abio, sed	8.42E+04				
S_bio_dead,sed	7.15E+03				
S_sed,total	9.14E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	4.63E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	6.80E+06	Link	
Q_out	Water Outflow	m3/yr	6.80E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	1.4	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	9.483249675	currently no exchange	
A12	interfacial area of epi/hyp	m	463365	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	5858941.314	modeled as 0	
Vw_1	Volume of Layer 1	m3	648711	Link	
Vw_2	Volume of Layer 2	m3	46336.5	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

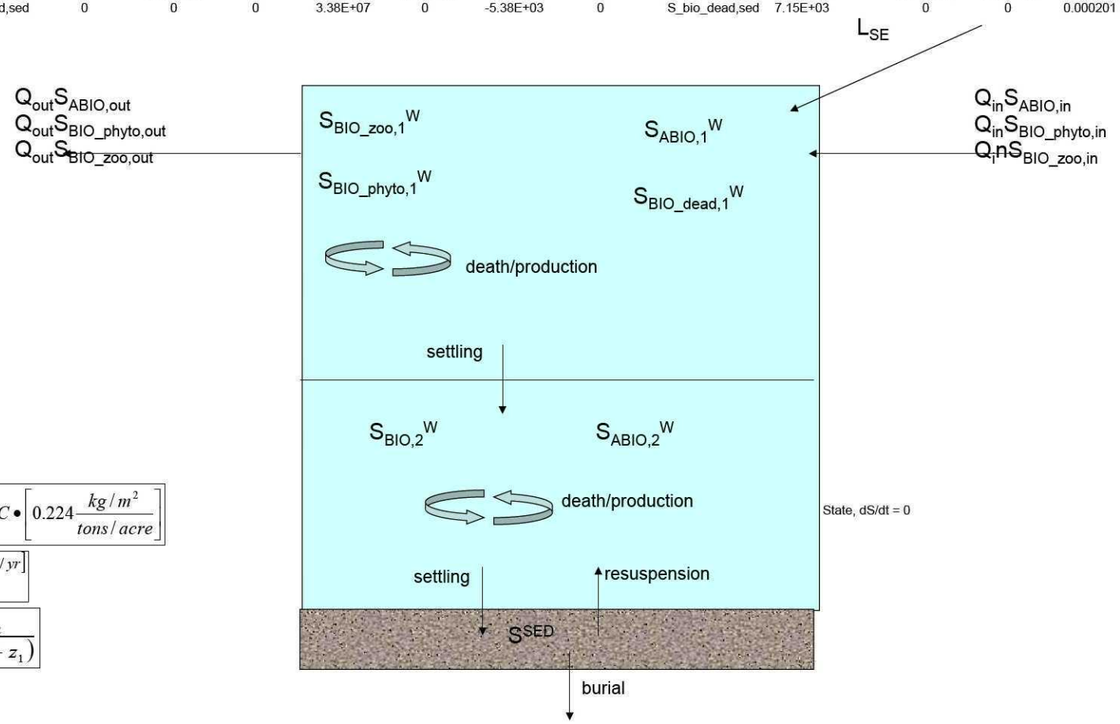
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	2.22E+09	5.86E+06	0	0	0	0	2.99E+08	S_abio,1	1.34E-01	4.48E-10	1.75E-12	0	0	5.72E-13	0	0.134084
S_abio,2	2.23E+09	-2.23E+09	0	0	1714.45282	0	0	S_abio,2	1.99E-01	6.65E-10	-6.64E-10	0	0	-2.2E-10	0	0.198936
S_bio_dead,1	0	0	3.48E+07	5.86E+06	0	0	3.55E+07	S_bio_dead,1	8.30E-01	0	0	2.34E-08	4.73E-09	0	1.51E-09	0.829741
S_bio_dead,2	0	0	3.97E+07	-3.97E+07	0	1.71E+03	0	S_bio_dead,2	1.14E+00	0	0	3.21E-08	-2.81E-08	0	-8.94E-09	1.138825
S_abio,sed	0	2.22E+09	0	0	-5.25E+03	0	0	S_abio,sed	8.42E+04	0.000282	-2.81E-04	0	0	-2.82E-04	0	84224.58
S_bio_dead,sed	0	0	0	3.38E+07	0	-5.38E+03	0	S_bio_dead,sed	7.15E+03	0	0	0.000201	-1.76E-04	0	-2.42E-04	7154.393



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00816	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.03612		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.03934		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.17421		
k_meth_1	abiotic methylation in layer 1		per yr	3.46E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	8.93E-06	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.16E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			3.61E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			3.93E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			1.74E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.02E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	8.93E-06	

$$k_{demeth} = k_{demeth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	1.78E-02	
k_photored_2	MeHg photored rate constant 2	per day	2.25E-03	
k_photored_1	MeHg photored rate constant 1	per year	6.51E+00	
k_photored_2	MeHg photored rate constant 2	per year	8.22E-01	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.27	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.03	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.04	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.31	
k_photoreduct_2	sum of vis + UV-B	per day	0.03	
k_photoreduct_1	sum of vis + UV-B	per yr	111.68	
k_photoreduct_2	sum of vis + UV-B	per yr	12.32	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.52	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	554.95	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	1.4	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	8.91	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	1.13E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	1.37E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	4.66E-49	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{1.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43* ,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	111.68	
k_photoreduct_2	sum of vis + UV-B		per yr	12.32	
k_net_reduction_1	net rate of reduction		per yr	122.63	
k_net_reduction_2	net rate of reduction		per yr	23.27	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Great Blue Heron

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations		
Hg0	0	g/m3
HgII	5.64E-06	g/m3
MeHg	7.33E-08	g/m3

Total Mercury Concentration in Contaminated Sediment, dry weight	40.7	ug/g

Known Mercury in Contaminated Soils		
Cs,Hg0	0	g/m3
Cs,HgII	1.129080624	g/m3
Cs,MeHg	4.13E-03	g/m3

Required Hazard Index for Sensitive Indicator	1

Kd_abio		
HgII	7,182,936	1
MeHg	15,887	1

Kd_bio		
HgII	17,941,378	1
MeHg	2,581,565	1

Kd_DOC		
HgII	301,427	1
MeHg	310,000	1

	PCT ERROR	CLEANUP
MeHg Filtered	3.65	10.87
HgT Filtered	-20.91	
MeHg Unfilter	-31.54	
HgT Unfiltere	244.41	
	5.64	48.90245623
	0.07332	75.12997546

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Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.58	ng/L		-15.58	-100	0.47	ng/L	4.37	ng/L
	HgII Filtered	2.97	ng/L		-2.97	-100	0.10	ng/L	0.84	ng/L
	MeHg Filtered	0.74	ng/L	0.77	0.03	3.6500678	0.04	ng/L	0.22	ng/L
	HgT Filtered	19.29	ng/L	15.26	-4.03	-20.91065	0.61	ng/L	5.43	ng/L
	Hg0 Unfiltered	15.58	ng/L		-15.58	-100	0.47	ng/L	4.37	ng/L
	HgII Unfiltered	57.66	ng/L		-57.66	-100	1.87	ng/L	16.26	ng/L
	MeHg Unfiltered	4.06	ng/L	2.78	-1.28	-31.54439	0.21	ng/L	1.20	ng/L
	HgT Unfiltered	77.30	ng/L	266.23	188.93	244.4148	2.55	ng/L	21.83	ng/L
Hypolimnion	Hg0 Filtered	110.39	ng/L		-110.39	-100	1.43	ng/L	29.54	ng/L
	HgII Filtered	244.01	ng/L		-244.01	-100	3.08	ng/L	65.23	ng/L
	MeHg Filtered	10.76	ng/L		-10.76	-100	0.29	ng/L	2.99	ng/L
	HgT Filtered	365.17	ng/L		-365.17	-100	4.79	ng/L	97.76	ng/L
	Hg0 Unfiltered	110.39	ng/L		-110.39	-100	1.43	ng/L	29.54	ng/L
	HgII Unfiltered	609.90	ng/L		-609.90	-100	7.69	ng/L	163.05	ng/L
	MeHg Unfiltered	12.80	ng/L		-12.80	-100	0.34	ng/L	3.56	ng/L
	HgT Unfiltered	733.10	ng/L		-733.10	-100	9.46	ng/L	196.14	ng/L
	Sediment									
	Hg0 porewater	110.39	ng/L		-110.39	-100	1.43	ng/L	29.541	ng/L
	HgII porewater	290.76	ng/L		-290.76	-100	3.60	ng/L	77.684	ng/L
	MeHg porewater	2.84	ng/L		-2.84	-100	0.06	ng/L	0.779	ng/L
	HgT porewater	403.99	ng/L		-403.99	-100	5.10	ng/L	108.003	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.65	ug/g		-40.65	-100	0.27	ug/g	10.86	ug/g
	MeHg bulk, dry	0.04611	ug/g	0.00658	-0.04	-85.72872	0.00	ug/g	0.01	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.505	ug/g	10.87	ug/g
Fish	Trophic Level 3	0.68	ug/g		-0.68	-100	0.035	ug/g	0.20	ug/g
	Trophic Level 4	1.48	ug/g		-1.48	-100	0.075	ug/g	0.44	ug/g
	HI	3.38					0.17		1.00	
	Sensitive Indicator	Great Blue Heron					Great Blue Heron		Great Blue Heron	
	Target C_sed, dry	10.87	ug/g	Note: 8						
	Target C_sed, wet	4.90	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.16E-07	per day	1.16E-04
	Hypolimnion	1.16E-06	per day	
	Sediment	3.49E-07	per day	
Demethylation	Epilimnion	1.16E-08	per day	
	Hypolimnion	1.16E-07	per day	
	Sediment	6.98E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

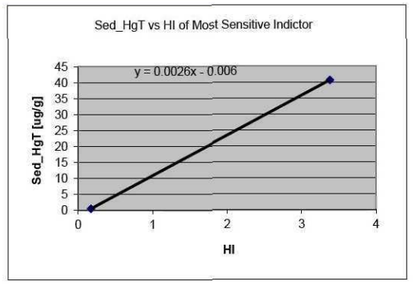
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.83	0.04	0.25
Otter	0.89	0.05	0.26
Mink	**1.74**	0.09	0.51
Great Blue Heron	**3.38**	0.17	**1.00**
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	**1.59**	0.08	0.47
Kingfisher	0.00	0.00	0.00
Wood Duck	0.62	0.03	0.18
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
3.38	40.70
0.17	0.50
m =	12.533
b=	-1.658
Sed_HgT	10.874
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under tools. Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

	Site-Specific User Input	Required
	Model Calculated	No input required
	Data Necessary for certain sites	Only necessary if applicable to site of interest
	Scenario 1 Output	
	Scenario 2 Output	
	Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.74	0.04	0.220	ng/L

Biota

Trophic Level 1: Phytoplankton	0.14	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Insects	0.12	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.13	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.68	0.03	0.20	ug Hg/ g wet weight
Trophic Level 4: Bass	1.48	0.08	0.44	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.80	0.04	0.24	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.14	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.13	0.01	0.04	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

	Wildlife Specific Parameters									Contaminated Sediment Calculations								
Animal	**Body Weight** [kg in wet weight]	**Ingestion Rate** [kg wet weight/d]	**Drinking rate** [L/d]	**Percent of Diet from Trophic Level 1 : Phytoplankton and Plants** --	**Percent of Diet from Trophic Level 2 : Insects** --	**Percent of Diet from Trophic Level 2 : Crayfish or Frogs** --	**Percent of Diet from Trophic Level 3 : Fish** --	**Percent of Diet from Trophic Level 4 : Fish** --	**Percent of Diet from nonaquatic sources** --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	62	0	0	0	62	75	0.83
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	2	50	15	67	75	0.89
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	6	5	119	130	75	**1.74**
Great Blue Heron	2.2	0.509	0.1	0%	5%	10%	50%	35%	0%	0	0	1	3	79	120	203	60	**3.38**
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	30	11	55	0	95	60	**1.59**
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	29	8	0	0	0	37	60	0.62
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	1	2	11	14	5000	0.00
Human	**Human Specific Parameters**																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.006	0.00	3.18	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.10	2.58	0.75	3	75	0.05
0.004	0.00	0.00	0.32	0.23	6.10	7	75	0.09
0.002	0.00	0.07	0.16	4.01	6.11	10	60	0.17
0.018	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.003	0.00	1.53	0.55	2.79	0.00	5	60	0.08
0.004	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.003	1.47	0.43	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.04	0.09	0.58	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.035	0.00	18.45	0.00	0.00	0.00	18	75	0.25
0.018	0.00	0.00	0.59	14.92	4.33	20	75	0.26
0.022	0.00	0.00	1.87	1.35	35.35	39	75	0.51
0.010	0.00	0.42	0.92	23.24	35.42	60	60	**1.00**
0.103	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.016	0.00	8.87	3.19	16.19	0.00	28	60	0.47
0.025	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.015	8.49	2.50	0.00	0.00	0.00	11	60	0.18
0.000	0.00	0.00	0.22	0.55	3.35	4	5000	0.00
							RfD	
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893.2	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.38

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.74E-07	0.47
C_HgII_1_Aq			g/m3	9.64E-08	0.10
C_MeHg_1_Aq			g/m3	3.79E-08	0.04
C_Hg0_2_Aq			g/m3	1.43E-06	1.43
C_HgII_2_Aq			g/m3	3.08E-06	3.08
C_MeHg_2_Aq			g/m3	2.86E-07	0.29
C_Hg0_pore			g/m3	1.43E-06	1.43
C_HgII_pore			g/m3	3.60E-06	3.60
C_MeHg_pore			g/m3	6.35E-08	0.06
C_HgT_1_filtered			g/m3	6.08E-07	0.61
C_HgT_2_filtered			g/m3	4.79E-06	4.79
C_HgT_Sed_filtered			g/m3	5.10E-06	5.10
C_Hg0_1_T			g/m3	4.74E-07	0.47
C_HgII_1_T			g/m3	1.87E-06	1.87
C_MeHg_1_T			g/m3	2.07E-07	0.21
C_Hg0_2_T			g/m3	1.43E-06	1.43
C_HgII_2_T			g/m3	7.69E-06	7.69
C_MeHg_2_T			g/m3	3.40E-07	0.34
C_Hg0_sed, bulk			g/m3	1.19E-06	1
C_HgII_1_sed, bulk			g/m3	2.27E-01	226,907
C_MeHg_1_sed, bulk			g/m3	4.65E-04	465
C_Hg0_sed, wet			g/g	9.27E-13	0.000
C_HgII_1_sed, wet			g/g	2.72E-07	0.272
C_MeHg_1_sed, wet			g/g	4.22E-14	0.000
C_HgT_sed,wet			g/g	2.72E-07	0.272
C_Hg0_sed, dry weight			g/g	2.63E-12	0.0000
C_HgII_1_sed, dry weight			g/g	5.04E-07	0.5037
C_MeHg_1_sed, dry weight			g/g	1.03E-09	0.0010
C_HgT_1			g/m3	2.55E-06	2.551
C_HgT_2			g/m3	9.46E-06	9.457
C_HgT_Sed, dry weight			g/g	5.05E-07	0.505

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)	8.13%	73.29%	18.58%
Layer 2		3.60%	81.28%	15.12%
Sediments		0.20%	99.80%	0.00%

Q'	Bulk Exchange Flow		m3/yr	3,017,619
Qin	Inflow		m3/yr	3,474,314
Qout	Outflow		m3/yr	3,474,314
Aw	Surface Area of the Water Body		m2	378,381
E	Exchange rate		m2/yr	2
V_1	Volume of Layer 1	Aw*z_1	m3	183,741
V_2	Volume of Layer 2	Aw*z_2	m3	37,838
z1	depth of first water layer		m	0.49
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.009
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.031
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.069
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.141
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.043
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.152
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.331
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.700

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored1} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{s2} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi}V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{s2} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg1}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{s2} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg1} + Q' \cdot C^w_{MeHg2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{s2} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{s2} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{s2} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{s2} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{s2} \cdot f^{w,2}_{bioHgII}\right) A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{s2} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed
	1	2	3	4	5	6	7	8	9
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.27E+08	0.00E+00	0.00E+00	-4.29E+03	2.89E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03

Matrix b

C_Hg0_1_T	-3.99E-01
C_HgII_1_T	-4.13E+01
C_MeHg_1_T	-9.97E-01
C_Hg0_2_T	0.00E+00
C_HgII_2_T	0.00E+00
C_MeHg_2_T	0.00E+00
C_Hg0_sed	0.00E+00
C_HgII_1_sed	0.00E+00
C_MeHg_1_sed	0.00E+00

Solution Matrix

C_Hg0_1_T	4.740E-07
C_HgII_1_T	1.870E-06
C_MeHg_1_T	2.074E-07
C_Hg0_2_T	1.430E-06
C_HgII_2_T	7.687E-06
C_MeHg_2_T	3.402E-07
C_Hg0_sed	1.187E-06
C_HgII_1_sed	2.269E-01
C_MeHg_1_sed	4.648E-04

Inverted Matrix

-1.21E-08	-1.12E-08	-5.13E-09	-1.14E-08	-1.13E-08	-5.60E-09	-1.14E-08	-1.13E-08	-5.60E-09
-2.70E-08	-4.47E-08	-1.21E-08	-3.98E-08	-4.17E-08	-1.42E-08	-3.98E-08	-4.17E-08	-1.42E-08
-7.21E-10	-1.15E-09	-1.60E-07	-2.55E-09	-2.83E-09	-1.48E-07	-2.55E-09	-2.88E-09	-1.48E-07
-2.197E-08	-3.407E-08	-1.369E-08	-1.17E-07	-8.15E-08	-2.15E-08	-1.17E-07	-8.14E-08	-2.15E-08
-1.147E-07	-1.835E-07	-6.226E-08	-4.06E-07	-4.50E-07	-8.83E-08	-4.06E-07	-4.50E-07	-8.85E-08
-2.334E-09	-3.731E-09	-1.856E-07	-8.26E-09	-9.16E-09	-4.79E-07	-8.26E-09	-9.32E-09	-4.78E-07
-1.82E-08	-2.83E-08	-1.14E-08	-9.73E-08	-6.76E-08	-1.78E-08	-4.02E-06	-6.76E-08	-1.79E-08
-3.39E-03	-5.42E-03	-1.84E-03	-1.20E-02	-1.33E-02	-2.61E-03	-1.20E-02	-1.35E-02	-2.61E-03
-3.80E-06	-6.08E-06	-2.13E-04	-1.35E-05	-1.49E-05	-5.48E-04	-1.35E-05	-1.52E-05	-7.79E-04

x=b/A

4.74001E-07
1.86967E-06
2.07388E-07
1.4299E-06
7.68731E-06
3.40213E-07
1.18682E-06
0.226906529
0.000464799

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.005
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.062
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.099
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.794
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.049
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.025
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.538
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.159
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		1.32E-05
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		1.13E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \quad \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS} = \frac{}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.58
C_HgII_1_Aq			g/m3	2.97E-06	2.97
C_MeHg_1_Aq			g/m3	7.43E-07	0.74
C_Hg0_2_Aq			g/m3	1.10E-04	110.39
C_HgII_2_Aq			g/m3	2.44E-04	244.01
C_MeHg_2_Aq			g/m3	1.08E-05	10.76
C_Hg0_pore			g/m3	1.10E-04	110.39
C_HgII_pore			g/m3	2.91E-04	290.76
C_MeHg_pore			g/m3	2.84E-06	2.84
C_HgT_1_filtered			g/m3	1.93E-05	19.29
C_HgT_2_filtered			g/m3	3.65E-04	365.17
C_HgT_Sed_filtered			g/m3	4.04E-04	403.99
C_Hg0_1_T			g/m3	1.56E-05	15.58
C_HgII_1_T			g/m3	5.77E-05	57.66
C_MeHg_1_T			g/m3	4.06E-06	4.06
C_Hg0_2_T			g/m3	1.10E-04	110.39
C_HgII_2_T			g/m3	6.10E-04	609.90
C_MeHg_2_T			g/m3	1.28E-05	12.80
C_Hg0_sed			g/m3	9.16E-05	91.63
C_HgII_1_sed			g/m3	1.83E+01	18314487.35
C_MeHg_1_sed			g/m3	2.08E-02	20771.02
C_Hg0_sed, wet			g/g	3.46E-11	0.000
C_HgII_1_sed, wet			g/g	1.43E-05	14.303
C_MeHg_1_sed, wet			g/g	2.49E-08	0.025
C_HgT_sed,wet			g/g	1.43E-05	14.328
C_Hg0_sed, dry weight			g/g	2.03E-10	0.00
C_HgII_1_sed, dry weight			g/g	4.07E-05	40.65
C_MeHg_1_sed, dry weight			g/g	4.61E-08	0.05
C_HgT_1			g/m3	7.73E-05	77.30
C_HgT_2			g/m3	7.33E-04	733.10
C_HgT_Sed			g/g	4.07E-05	40.70
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		5.25%	74.59%	20.15%
Layer 2			1.75%	83.19%	15.06%
Sediments			0.11%	99.89%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.88548%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	3.06930%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	6.87088%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	4.27053%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	15.22372%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	33.13706%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.02796%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{Hg1,1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg,1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{Hg1,1}}{dt} = L_{T,Hg1,1} + Q_{in} C_{in,Hg1,1} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg,1} + \left[-Q_{out} - Q' - kw_{volHg1,1} \cdot V_w - kw_{red,1} \cdot V_w - kw_{metR} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abioHg1,1} A_w - v_{sB} \cdot f^{w,1}_{bioHg1,1} A_w\right] \cdot C^w_{Hg1,1} + Q' \cdot C^w_{Hg1,2}$$

$$V_w \frac{dC^w_{MeHg,1}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{metR} \cdot V_w\right] \cdot C^w_{Hg1,1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s,1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg,1} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red,2} \cdot V_w\right] \cdot C^w_{Hg1,2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg,2} + \left[-Q' - kw_{oxid} V_w - v_{s,1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{Hg1,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg,2} + \left[-Q' - kw_{red,2} \cdot V_w - kw_{metR} \cdot V_w - v_{s,1} \cdot f^{w,2}_{abioHg1,1} A_w - v_{sB} \cdot f^{w,2}_{bioHg1,1} A_w - R_{sw} \cdot f^{w,2}_{aqHg1,1}\right] \cdot C^w_{Hg1,2} + Q' \cdot C^w_{Hg1,3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg1,1}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg1,1} A_w\right] \cdot C^{sed}_{aqHg1,1}$$

$$V_w \frac{dC^w_{MeHg,2}}{dt} = +\left[kw_{metR2} \cdot V_w\right] \cdot C^w_{Hg1,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s,1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg,2} + Q' \cdot C^w_{MeHg,3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.57E-01	C_MeHg_1_T
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix										x=b/A
1.558E-05	-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.34E-07	-2.77E-09	1.56E-05	
5.766E-05	-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.78E-09	5.77E-05	
4.061E-06	-9.27E-17	-3.53E-16	-1.59E-07	7.27E-15	-4.95E-16	-1.47E-07	8.42E-13	2.13E-07	-1.47E-07	4.06E-06	
1.104E-04	-1.569E-09	-1.446E-09	-1.353E-09	4.51E-08	-1.40E-09	-2.51E-09	-4.51E-08	6.02E-06	-1.11E-09	0.00011	
6.099E-04	-1.979E-09	-3.165E-09	5.934E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.33E-05	2.43E-08	0.00061	
1.280E-05	7.949E-17	-4.998E-16	-1.842E-07	2.36E-14	-1.59E-15	-4.76E-07	2.72E-12	6.88E-07	-4.76E-07	1.28E-05	
9.163E-05	-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.20E-10	9.16E-05	
1.831E+01	1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.44E-04	3.95E-06	9.99E-01	7.75E-04	18.31449	
2.077E-02	5.27E-13	-1.69E-13	-2.10E-04	3.95E-11	-1.42E-12	-5.44E-04	4.44E-09	1.12E-03	-7.75E-04	0.020771	

A*x=b

C_T_sed 18.33535 g/m3

$$C^{sed}_{dry.}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	7.90
TSS+2			mg/L	0.56
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_Hg0_1	Effective K for Hg0 in layer 2		L/kg	2.33E+06
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.66E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	3.37E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.37E-06	4.37
C_HgII_1_Aq			g/m3	8.38E-07	0.84
C_MeHg_1_Aq			g/m3	2.20E-07	0.22
C_Hg0_2_Aq			g/m3	2.95E-05	29.54
C_HgII_2_Aq			g/m3	6.52E-05	65.23
C_MeHg_2_Aq			g/m3	2.99E-06	2.99
C_Hg0_pore			g/m3	2.95E-05	29.54
C_HgII_pore			g/m3	7.77E-05	77.68
C_MeHg_pore			g/m3	7.79E-07	0.78
C_HgT_1_filtered			g/m3	5.43E-06	5.43
C_HgT_2_filtered			g/m3	9.78E-05	97.76
C_HgT_Sed_filtered			g/m3	1.08E-04	108.00
C_Hg0_1_T			g/m3	4.37E-06	4.37
C_HgII_1_T			g/m3	1.63E-05	16.26
C_MeHg_1_T			g/m3	1.20E-06	1.20
C_Hg0_2_T			g/m3	2.95E-05	29.54
C_HgII_2_T			g/m3	1.63E-04	163.05
C_MeHg_2_T			g/m3	3.56E-06	3.56
C_Hg0_sed			g/m3	2.45E-05	24.52
C_HgII_1_sed			g/m3	4.89E+00	4,893,169.85
C_MeHg_1_sed			g/m3	5.70E-03	5,703.43
C_Hg0_sed, wet			g/g	9.25E-12	0.00
C_HgII_1_sed, wet			g/g	3.82E-06	3.82
C_MeHg_1_sed, wet			g/g	6.83E-09	0.01
C_HgT_sed,wet			g/g	3.83E-06	3.83
C_Hg0_sed, dry weight			g/g	5.44E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.09E-05	10.86
C_MeHg_1_sed, dry weight			g/g	1.27E-08	0.01
C_HgT_1			g/m3	2.18E-05	21.83
C_HgT_2			g/m3	1.96E-04	196.14
C_HgT_Sed, dry weight			g/g	1.09E-05	10.87
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		5.50%	74.48%	20.02%
Layer 2			1.81%	83.13%	15.06%
Sediments			0.12%	99.88%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			4.27053%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			33.13706%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	4.371E-06	-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.34E-07	-2.77E-09	4.4E-06
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.626E-05	-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.78E-09	1.6E-05
C_MeHg_1_T	0.00E+00	6.81E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	1.202E-06	-9.27E-17	-3.53E-16	-1.59E-07	7.27E-15	-4.95E-16	-1.47E-07	8.42E-13	2.13E-07	-1.47E-07	1.2E-06
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	2.954E-05	-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.51E-09	-4.51E-08	6.02E-06	-1.11E-09	3E-05
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	1.630E-04	-1.979E-09	-3.165E-09	5.934E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.33E-05	2.43E-08	0.00016
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T	3.556E-06	7.949E-17	-4.998E-16	-1.842E-07	2.36E-14	-1.59E-15	-4.76E-07	2.72E-12	6.88E-07	-4.76E-07	3.6E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	2.452E-05	-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.20E-10	2.5E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	4.90E+00	C_HgII_1_sed	4.893E+00	1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.44E-04	3.95E-06	9.99E-01	7.75E-04	4.89317
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	5.703E-03	5.27E-13	-1.69E-13	-2.10E-04	3.95E-11	-1.42E-12	-5.44E-04	4.44E-09	1.12E-03	-7.75E-04	0.0057

A*x=b

Target C_sed, wet 4.898897797 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	388.36
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	246.95
kw_red_2	water column reduction rate constant	per yr	107.40
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for	per yr	6.43
kw_mer	water column *mer* cleavage demeth	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

$$kw_{v,i} = \frac{K_{v,1} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{}{C_{diss,i}^j + C_{DOC,i}^j} \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- =	Total Chloride
SO_4^{2-} =	Total Sulfate
S^{2-} =	Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27053%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			33.13706%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.53471%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			6.15876%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00410%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.92923%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			79.43383%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			4.94622%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			53.83330%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			2.46695%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.98867%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.31
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.44
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	2,743.46
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	7.90	mg/L
Sbio_zoo,1	2.5		TSS_2	0.56	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	3.11E-01				
Sbio_dead,2	4.37E-01				
S_abio, sed	5.28E+04				
S_bio_dead,sed	2.74E+03				
S_sed,total	5.56E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

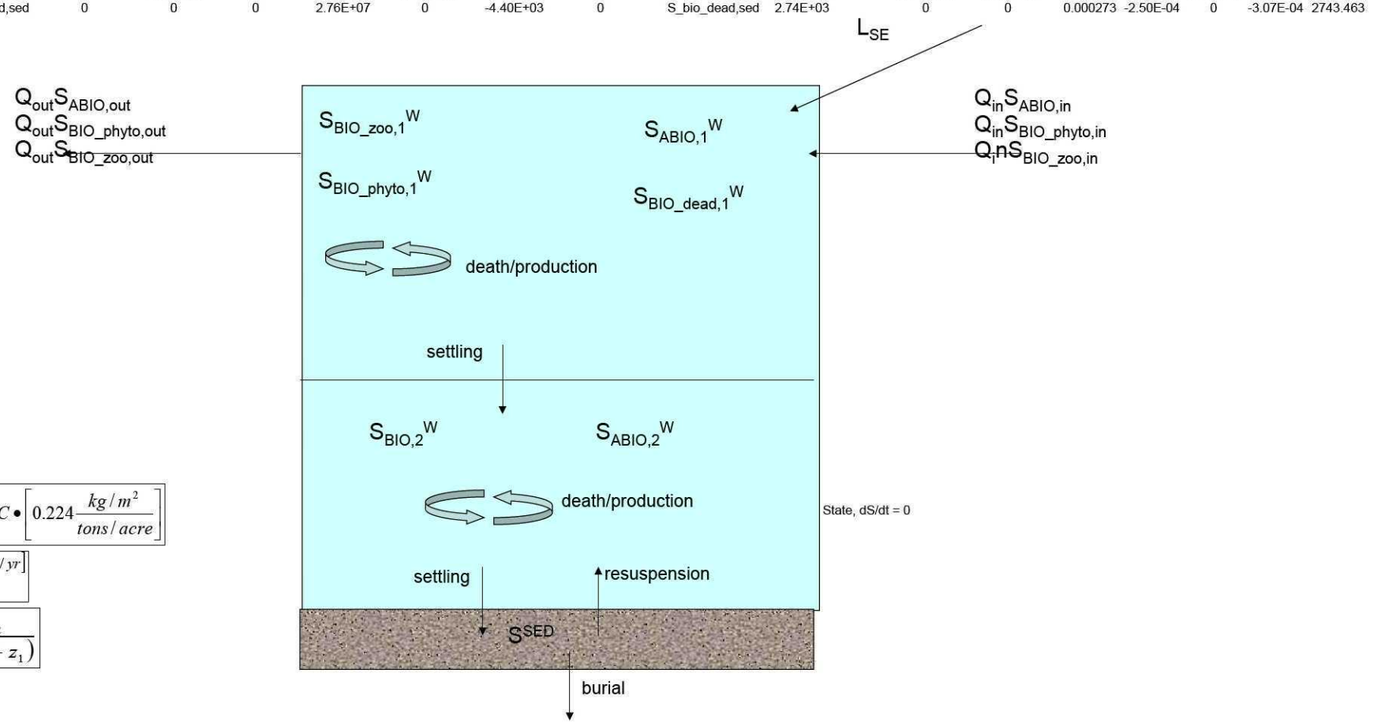
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	1.01E+07	S_bio_dead,1	3.11E-01	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.311342
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	4.37E-01	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.4367
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	2.74E+03	0	0	0.000273	-2.50E-04	0	-3.07E-04	2743.463



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00885	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.06871		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.04271		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.33137		
k_meth_1	abiotic methylation in layer 1		per yr	3.76E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.70E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.85E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			3.31E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.19E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.70E-05	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43* ,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Pied-Billed Grebe

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3			
HgII	5.64E-06	g/m3	5.64	35.58437977	
MeHg	7.33E-08	g/m3	0.07332	83.29934922	Fish

Total Mercury Concentration in Contaminated Sediment, dry weight	40.7	ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Exposure Concentrations

	Kd_abio			
	HgII	7,182,936	1	
	MeHg	15,887	1	
	Kd_bio			
	HgII	17,941,378	1	
	MeHg	2,581,565	1	
	Kd_DOC			
	HgII	301,427	1	
	MeHg	310,000	1	
		PCT ERROR	CLEANUP	
	MeHg Filtered	-23.71	18.18	
	HgT Filtered	-22.10		
	MeHg Unfilter	-49.61		
	HgT Unfiltere	237.77		

		Scenario 1 With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2 Background Conditions		Scenario 3 Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.61	ng/L		-15.61	-100	0.47	ng/L	7.13	ng/L
	HgII Filtered	2.97	ng/L		-2.97	-100	0.10	ng/L	1.36	ng/L
	MeHg Filtered	1.01	ng/L	0.77	-0.24	-23.71046	0.04	ng/L	0.47	ng/L
	HgT Filtered	19.59	ng/L	15.26	-4.33	-22.10485	0.61	ng/L	8.96	ng/L
	Hg0 Unfiltered	15.61	ng/L		-15.61	-100	0.47	ng/L	7.13	ng/L
	HgII Unfiltered	57.70	ng/L		-57.70	-100	1.87	ng/L	26.41	ng/L
	MeHg Unfiltered	5.52	ng/L	2.78	-2.74	-49.61463	0.23	ng/L	2.55	ng/L
	HgT Unfiltered	78.82	ng/L	266.23	187.41	237.76746	2.56	ng/L	36.09	ng/L
Hypolimnion	Hg0 Filtered	110.40	ng/L		-110.40	-100	1.42	ng/L	49.34	ng/L
	HgII Filtered	243.91	ng/L		-243.91	-100	3.06	ng/L	108.96	ng/L
	MeHg Filtered	14.72	ng/L		-14.72	-100	0.33	ng/L	6.66	ng/L
	HgT Filtered	369.04	ng/L		-369.04	-100	4.81	ng/L	164.97	ng/L
	Hg0 Unfiltered	110.40	ng/L		-110.40	-100	1.42	ng/L	49.34	ng/L
	HgII Unfiltered	609.66	ng/L		-609.66	-100	7.64	ng/L	272.35	ng/L
	MeHg Unfiltered	17.52	ng/L		-17.52	-100	0.40	ng/L	7.92	ng/L
	HgT Unfiltered	737.58	ng/L		-737.58	-100	9.46	ng/L	329.62	ng/L
	Sediment									
	Hg0 porewater	110.40	ng/L		-110.40	-100	1.42	ng/L	49.342	ng/L
	HgII porewater	290.64	ng/L		-290.64	-100	3.58	ng/L	129.800	ng/L
	MeHg porewater	3.88	ng/L		-3.88	-100	0.08	ng/L	1.750	ng/L
	HgT porewater	404.93	ng/L		-404.93	-100	5.08	ng/L	180.893	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.64	ug/g		-40.64	-100	0.27	ug/g	18.15	ug/g
	MeHg bulk, dry	0.06314	ug/g	0.00658	-0.06	-89.57908	0.00	ug/g	0.03	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.502	ug/g	18.18	ug/g
	Trophic Level 3	0.92	ug/g		-0.92	-100	0.038	ug/g	0.43	ug/g
	Trophic Level 4	2.01	ug/g		-2.01	-100	0.082	ug/g	0.93	ug/g
	HI	2.16					0.09		1.00	
	Sensitive Indicator	Pied-bill Grebe					Pied-bill Grebe		Pied-bill Grebe	
	Target C_sed, dry	18.18	ug/g	Note: 8						
	Target C_sed, wet	8.19	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.60E-07	per day	1.60E-04
	Hypolimnion	1.60E-06	per day	
	Sediment	4.80E-07	per day	
Demethylation	Epilimnion	1.60E-08	per day	
	Hypolimnion	1.60E-07	per day	
	Sediment	9.60E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

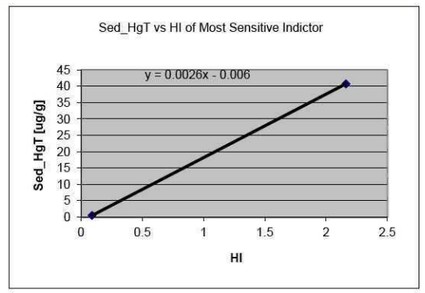
Human and Wildlife Exposure Risk Results

6,250

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	1.13	0.05	0.52
Otter	1.22	0.05	0.56
Mink	0.00	0.00	0.00
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	2.16	0.09	1.00
Kingfisher	0.00	0.00	0.00
Wood Duck	0.84	0.03	0.39
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
2.16	40.70
0.09	0.50
m =	19.384
b=	-1.207
Sed_HgT	18.177
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	1.01	0.04	0.467	ng/L

Biota

Trophic Level 1: Phytoplankton	0.19	0.01	0.09	ug Hg/ g wet weight
Trophic Level 2: Insects	0.17	0.01	0.08	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.18	0.01	0.08	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.92	0.04	0.43	ug Hg/ g wet weight
Trophic Level 4: Bass	2.01	0.08	0.93	ug Hg/ g wet weight
Trophic Level 3: Silverside	1.09	0.04	0.50	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.19	0.01	0.09	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.18	0.01	0.08	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Body Weight	Ingestion Rate	Drinking rate	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants	Percent of Diet from Trophic Level 2 : Insects	Percent of Diet from Trophic Level 2 : Crayfish or Frogs	Percent of Diet from Trophic Level 3 : Fish	Percent of Diet from Trophic Level 4 : Fish	Percent of Diet from nonaquatic sources	Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Insects	Potential Dose from Trophic Level 2: Crayfish	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
Animal	[kg in wet weight]	[kg wet weight/d]	[L/d]	--	--	--	--	--	--	[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	85	0	0	0	85	75	**1.13**
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	3	69	20	91	75	**1.22**
Mink	0.85	0.1145	0.085	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	75	0.00
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	41	15	74	0	130	60	**2.16**
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	39	11	0	0	0	50	60	0.84
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	1	3	15	19	5000	0.00
Human																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.007	0.00	3.46	0.00	0.00	0.00	3	75	0.05
0.003	0.00	0.00	0.11	2.80	0.81	4	75	0.05
0.004	0.00	0.00	0.00	0.00	0.00	0	75	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.019	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.003	0.00	1.66	0.60	3.03	0.00	5	60	0.09
0.005	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.003	1.59	0.47	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.04	0.10	0.63	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.075	0.00	39.19	0.00	0.00	0.00	39	75	0.52
0.039	0.00	0.00	1.25	31.70	9.20	42	75	0.56
0.047	0.00	0.00	0.00	0.00	0.00	0	75	0.00
0.021	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.220	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.034	0.00	18.85	6.77	34.38	0.00	60	60	**1.00**
0.053	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.031	18.03	5.31	0.00	0.00	0.00	23	60	0.39
0.000	0.00	0.00	0.47	1.16	7.12	9	5000	0.00
							RfD	
0.008	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Pied-Billed Grebe

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes			Oligo	Meso	Eutro	Dystro	
1	Trophic Status is determined DOC in Epiliminon as:		<3	3-5	5-10	10+	mg DOC/L
	from Wetzel	Flag	1	2	3	4	
2	Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.73E-07	0.47
C_HgII_1_Aq			g/m3	9.62E-08	0.10
C_MeHg_1_Aq			g/m3	4.12E-08	0.04
C_Hg0_2_Aq			g/m3	1.42E-06	1.42
C_HgII_2_Aq			g/m3	3.06E-06	3.06
C_MeHg_2_Aq			g/m3	3.34E-07	0.33
C_Hg0_pore			g/m3	1.42E-06	1.42
C_HgII_pore			g/m3	3.58E-06	3.58
C_MeHg_pore			g/m3	7.62E-08	0.08
C_HgT_1_filtered			g/m3	6.11E-07	0.61
C_HgT_2_filtered			g/m3	4.81E-06	4.81
C_HgT_Sed_filtered			g/m3	5.08E-06	5.08
C_Hg0_1_T			g/m3	4.73E-07	0.47
C_HgII_1_T			g/m3	1.87E-06	1.87
C_MeHg_1_T			g/m3	2.25E-07	0.23
C_Hg0_2_T			g/m3	1.42E-06	1.42
C_HgII_2_T			g/m3	7.64E-06	7.64
C_MeHg_2_T			g/m3	3.97E-07	0.40
C_Hg0_sed, bulk			g/m3	1.18E-06	1
C_HgII_1_sed, bulk			g/m3	2.26E-01	225,579
C_MeHg_1_sed, bulk			g/m3	5.58E-04	558
C_Hg0_sed, wet			g/g	9.22E-13	0.000
C_HgII_1_sed, wet			g/g	2.70E-07	0.270
C_MeHg_1_sed, wet			g/g	5.07E-14	0.000
C_HgT_sed,wet			g/g	2.70E-07	0.270
C_Hg0_sed, dry weight			g/g	2.62E-12	0.0000
C_HgII_1_sed, dry weight			g/g	5.01E-07	0.5007
C_MeHg_1_sed, dry weight			g/g	1.24E-09	0.0012
C_HgT_1			g/m3	2.56E-06	2.565
C_HgT_2			g/m3	9.46E-06	9.463
C_HgT_Sed, dry weight			g/g	5.02E-07	0.502
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		8.77%	72.77%	18.45%
Layer 2			4.20%	80.77%	15.03%
Sediments			0.25%	99.75%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.009
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.031
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.069
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.141
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.043
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.152
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.331
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.700

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored1} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi1} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg1}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg1} + Q' \cdot C^w_{MeHg2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,A} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sed,Hg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,A} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,A} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bio,MeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sed,MeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	4.733E-07	-1.21E-08	-1.12E-08	-5.12E-09	-1.14E-08	-1.13E-08	-5.59E-09	-1.14E-08	-1.12E-08	-5.60E-09	4.73309E-07
C_HgII_1_T	1.12E+08	-6.29E+07	5.53E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.866E-06	-2.70E-08	-4.46E-08	-1.21E-08	-3.96E-08	-4.15E-08	-1.42E-08	-3.96E-08	-4.15E-08	-1.42E-08	1.86633E-06
C_MeHg_1_T	0.00E+00	9.50E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	2.250E-07	-9.85E-10	-1.58E-09	-1.60E-07	-3.49E-09	-3.87E-09	-1.48E-07	-3.49E-09	-3.93E-09	-1.48E-07	2.25039E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.423E-06	-2.186E-08	-3.389E-08	-1.365E-08	-1.17E-07	-8.10E-08	-2.14E-08	-1.17E-07	-8.10E-08	-2.15E-08	1.42261E-06
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	8.84E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	7.643E-06	-1.141E-07	-1.824E-07	-6.198E-08	-4.04E-07	-4.48E-07	-8.80E-08	-4.04E-07	-4.47E-07	-8.83E-08	7.64329E-06
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	8.84E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T	3.973E-07	-3.187E-09	-5.096E-09	-1.859E-07	-1.13E-08	-1.25E-08	-4.79E-07	-1.13E-08	-1.27E-08	-4.78E-07	3.97302E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	1.181E-06	-1.81E-08	-2.81E-08	-1.13E-08	-9.70E-08	-6.73E-08	-1.78E-08	-4.02E-06	-6.72E-08	-1.78E-08	1.18076E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.27E+08	0.00E+00	0.00E+00	-4.29E+03	3.98E+00	0.00E+00	C_HgII_1_sed	2.256E-01	-3.37E-03	-5.38E-03	-1.83E-03	-1.19E-02	-1.32E-02	-2.60E-03	-1.19E-02	-1.34E-02	-2.61E-03	0.225578848
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.99E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	5.578E-04	-5.19E-06	-8.30E-06	-2.13E-04	-1.84E-05	-2.04E-05	-5.48E-04	-1.84E-05	-2.07E-05	-7.80E-04	0.000557807

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.005
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			0.062
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			0.099
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			0.396
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			0.794
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			0.396
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			0.049
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			0.025
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			0.538
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			0.159
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			1.32E-05
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			1.13E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			1.00E+00
L_T,Hg0	Total Load, Hg0		g/yr	3.99E-01
L_T,HgII	Total Load, HgII		g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg		g/yr	7.43E-01
Rate Constants				
kw_v,Hg0	water column volatilization loss rate constant, Hg0		per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII		per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg		per yr	0.65
kw_oxid_1	water column oxidation rate constant		per yr	610.22
kw_oxid_2	water column oxidation rate constant		per yr	525.60
kw_red_1	water column reduction rate constant, layer 2		per yr	246.95
kw_red_2	water column reduction rate constant, layer 2		per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1		per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2		per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1		per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2		per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1		per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2		per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant		per yr	0.00
kb_oxid	benthic oxidation rate constant		per yr	0.00
kb_red	benthic reduction rate constant		per yr	0.00
kb_methy	benthic methylation rate constant		per yr	0.00
kb_demeth	benthic demethylation rate constant		per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant		per yr	0.00
v_sA	abiotic settling velocity		m/yr	4,792.63
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.030
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	7.90
TSS+2			mg/L	0.56
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1		L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2		L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2		L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	3.37E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \quad \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS} = \frac{}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.61
C_HgII_1_Aq			g/m3	2.97E-06	2.97
C_MeHg_1_Aq			g/m3	1.01E-06	1.01
C_Hg0_2_Aq			g/m3	1.10E-04	110.40
C_HgII_2_Aq			g/m3	2.44E-04	243.91
C_MeHg_2_Aq			g/m3	1.47E-05	14.72
C_Hg0_pore			g/m3	1.10E-04	110.40
C_HgII_pore			g/m3	2.91E-04	290.64
C_MeHg_pore			g/m3	3.88E-06	3.88
C_HgT_1_filtered			g/m3	1.96E-05	19.59
C_HgT_2_filtered			g/m3	3.69E-04	369.04
C_HgT_Sed_filtered			g/m3	4.05E-04	404.93
C_Hg0_1_T			g/m3	1.56E-05	15.61
C_HgII_1_T			g/m3	5.77E-05	57.70
C_MeHg_1_T			g/m3	5.52E-06	5.52
C_Hg0_2_T			g/m3	1.10E-04	110.40
C_HgII_2_T			g/m3	6.10E-04	609.66
C_MeHg_2_T			g/m3	1.75E-05	17.52
C_Hg0_sed			g/m3	9.16E-05	91.64
C_HgII_1_sed			g/m3	1.83E+01	18306812.78
C_MeHg_1_sed			g/m3	2.84E-02	28445.58
C_Hg0_sed, wet			g/g	3.46E-11	0.000
C_HgII_1_sed, wet			g/g	1.43E-05	14.297
C_MeHg_1_sed, wet			g/g	3.41E-08	0.034
C_HgT_sed,wet			g/g	1.43E-05	14.331
C_Hg0_sed, dry weight			g/g	2.03E-10	0.00
C_HgII_1_sed, dry weight			g/g	4.06E-05	40.64
C_MeHg_1_sed, dry weight			g/g	6.31E-08	0.06
C_HgT_1			g/m3	7.88E-05	78.82
C_HgT_2			g/m3	7.38E-04	737.58
C_HgT_Sed			g/g	4.07E-05	40.70

			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		7.00%	73.20%	19.80%
Layer 2			2.37%	82.66%	14.97%
Sediments			0.16%	99.84%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.88548%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	3.06930%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	6.87088%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	4.27053%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	15.22372%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	33.13706%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.02796%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg1} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{metlR} \cdot V_w - v_{s1} \cdot f^{w,1}_{abiHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg1}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{metlB} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg1} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg2} + \left[-Q' - kw_{red2} \cdot V_w - kw_{metlR} \cdot V_w - v_{s1} \cdot f^{w,2}_{abiHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{metal2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2} + Q' \cdot C^w_{MeHg1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w}{\theta_{sed}}\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C Hg0 1 T	C HgII 1 T	C MeHg 1 T	C Hg0 2 T	C HgII 2 T	C MeHg 2 T	C Hg0 1 sed	C HgII 1 sed	C MeHg 1 sed	Matrix b	
	1	2	3	4	5	6	7	8	9		
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T
C_HgII_1_T	1.12E+08	-6.29E+07	5.53E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	9.50E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.57E-01	C_MeHg_1_T
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	8.84E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	8.84E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.99E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix											x=b/A
1.561E-05	-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.36E-07	-2.77E-09	1.56E-05		
5.770E-05	-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.77E-09	5.77E-05		
5.517E-06	-1.28E-16	-4.85E-16	-1.59E-07	9.98E-15	-6.81E-16	-1.47E-07	1.16E-12	2.92E-07	-1.47E-07	5.52E-06		
1.104E-04	-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.50E-09	-4.51E-08	6.02E-06	-1.11E-09	0.00011		
6.097E-04	-1.979E-09	-3.165E-09	5.926E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.32E-05	2.43E-08	0.00061		
1.752E-05	1.087E-16	-6.871E-16	-1.840E-07	3.24E-14	-2.18E-15	-4.76E-07	3.74E-12	9.45E-07	-4.75E-07	1.75E-05		
9.164E-05	-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.19E-10	9.16E-05		
1.831E+01	1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.43E-04	3.95E-06	9.98E-01	7.74E-04	18.30681		
2.845E-02	7.24E-13	-2.32E-13	-2.10E-04	5.42E-11	-1.95E-12	-5.43E-04	6.09E-09	1.54E-03	-7.74E-04	0.028446		

A*x=b

C T sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	orgaanic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	orgaanic particulate phase fraction of HgII in water column, layer 1		4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		2.46695%
f_org_Hg0_w_2	orgaanic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	orgaanic particulate phase fraction of HgII in water column, layer 2		53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity		m/yr		4792.628412
v_sB	biotic settling velocity		m/yr		73
v_rs	resuspension velocity		m/yr		0.003700005
k_mort	phytoplankton mortality rate		per yr		10.95
v_min	mineralization rate		per yr		0.01
v_bur	burial rate		m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0			m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII			m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg			m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0			m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII			m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg			m2/sec	6.11E-10
rho_s	Sediment Particle Density			g/cm3	2.65E+00
θ_sed	sediment porosity			cm3/cm3	0.83
z_sed	sediment layer,char mixing length			m	0.03
V_sed	Volume of Sediment	Aw*z_sed		m3	11351.43
TSS_1				mg/L	7.90
TSS+2				mg/L	0.56
Effective Partition Coefficients for each Hg species and layer					
K_eff_Hg0_1	Effective K for Hg0 in layer 1			L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2			L/kg	2.33E+06
K_eff_MeHg_1	Effective K for HgII in layer 1			L/kg	5.66E+05
K_eff_Hg0_2	Effective K for HgII in layer 2			L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1			L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2			L/kg	3.37E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	7.13E-06	7.13
C_HgII_1_Aq			g/m3	1.36E-06	1.36
C_MeHg_1_Aq			g/m3	4.67E-07	0.47
C_Hg0_2_Aq			g/m3	4.93E-05	49.34
C_HgII_2_Aq			g/m3	1.09E-04	108.96
C_MeHg_2_Aq			g/m3	6.66E-06	6.66
C_Hg0_pore			g/m3	4.93E-05	49.34
C_HgII_pore			g/m3	1.30E-04	129.80
C_MeHg_pore			g/m3	1.75E-06	1.75
C_HgT_1_filtered			g/m3	8.96E-06	8.96
C_HgT_2_filtered			g/m3	1.65E-04	164.97
C_HgT_Sed_filtered			g/m3	1.81E-04	180.89
C_Hg0_1_T			g/m3	7.13E-06	7.13
C_HgII_1_T			g/m3	2.64E-05	26.41
C_MeHg_1_T			g/m3	2.55E-06	2.55
C_Hg0_2_T			g/m3	4.93E-05	49.34
C_HgII_2_T			g/m3	2.72E-04	272.35
C_MeHg_2_T			g/m3	7.92E-06	7.92
C_Hg0_sed			g/m3	4.10E-05	40.95
C_HgII_1_sed			g/m3	8.18E+00	8,175,900.49
C_MeHg_1_sed			g/m3	1.28E-02	12,820.07
C_Hg0_sed, wet			g/g	1.55E-11	0.00
C_HgII_1_sed, wet			g/g	6.38E-06	6.38
C_MeHg_1_sed, wet			g/g	1.54E-08	0.02
C_HgT_sed,wet			g/g	6.40E-06	6.40
C_Hg0_sed, dry weight			g/g	9.09E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.81E-05	18.15
C_MeHg_1_sed, dry weight			g/g	2.85E-08	0.03
C_HgT_1			g/m3	3.61E-05	36.09
C_HgT_2			g/m3	3.30E-04	329.62
C_HgT_Sed, dry weight			g/g	1.82E-05	18.18
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		7.07%	73.18%	19.75%
Layer 2			2.40%	82.63%	14.97%
Sediments			0.16%	99.84%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
z2	depth of second water layer		m	0	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.88548%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	3.06930%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	6.87088%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	4.27053%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	15.22372%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	33.13706%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	69.96409%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photoredd} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abiHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoredd} V_w - v_{s1} \cdot f^{w,1}_{abiMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photoredd} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abiHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abiHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoredd} \cdot V_w - v_{s1} \cdot f^{w,2}_{abiMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{s1} \cdot f^{w,2}_{abiaHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{s1} \cdot f^{w,2}_{abiHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{s1} \cdot f^{w,2}_{abiaMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A

	C_Hg0_1_T	C_HgII_1_T	C_MeHg_1_T	C_Hg0_2_T	C_HgII_2_T	C_MeHg_2_T	C_Hg0_1_sed	C_HgII_1_sed	C_MeHg_1_sed
	1	2	3	4	5	6	7	8	9
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_HgII_1_T	1.12E+08	-6.29E+07	5.53E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
C_MeHg_1_T	0.00E+00	9.50E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	8.84E-01	0.00E+00	4.29E+03	0.00E+00
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	8.84E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.99E+00	-4.31E+03

A*x=b

Matrix b

C_Hg0_1_T	-3.99E-01
C_HgII_1_T	-4.13E+01
C_MeHg_1_T	-9.97E-01
C_Hg0_2_T	0.00E+00
C_HgII_2_T	0.00E+00
C_MeHg_2_T	0.00E+00
C_Hg0_sed	0.00E+00
C_HgII_1_sed	8.19E+00
C_MeHg_1_sed	0.00E+00

Target C_sed, wet 8.188761515 g/g

Solution Matrix

C_Hg0_1_T	7.127E-06
C_HgII_1_T	2.641E-05
C_MeHg_1_T	2.552E-06
C_Hg0_2_T	4.934E-05
C_HgII_2_T	2.724E-04
C_MeHg_2_T	7.924E-06
C_Hg0_sed	4.095E-05
C_HgII_1_sed	8.176E+00
C_MeHg_1_sed	1.282E-02

Inverted Matrix

-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.36E-07	-2.77E-09	7.13E-06
-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.77E-09	2.64E-05
-1.28E-16	-4.85E-16	-1.59E-07	9.98E-15	-6.81E-16	-1.47E-07	1.16E-12	2.92E-07	-1.47E-07	2.55E-06
-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.50E-09	-4.51E-08	6.02E-06	-1.11E-09	4.93E-05
-1.979E-09	-3.165E-09	5.926E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.32E-05	2.43E-08	0.000272
1.087E-16	-6.871E-16	-1.840E-07	3.24E-14	-2.18E-15	-4.76E-07	3.74E-12	9.45E-07	-4.75E-07	7.92E-06
-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.19E-10	4.1E-05
1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.43E-04	3.95E-06	9.98E-01	7.74E-04	8.1759
7.24E-13	-2.32E-13	-2.10E-04	5.42E-11	-1.95E-12	-5.43E-04	6.09E-09	1.54E-03	-7.74E-04	0.01282

x=b/A

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	orqanic particulate phase fraction of HqII in water column, layer 1		4.94622%
f_org_MeHg_w_1	orqanic particulate phase fraction of MeHq in water column, layer 1		2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	orqanic particulate phase fraction of HqII in water column, layer 2		53.83330%
f_org_MeHg_w_2	orqanic particulate phase fraction of MeHq in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatiilization loss rate cc	per yr	388.36
kw_v,HgII	water column volatiilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatiilization loss rate cc	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	246.95
kw_red_2	water column reduction rate constant,	per yr	107.40
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for I	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for I	per yr	6.43
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \times 10^7$$

$$K_{eff,i}^j = \frac{\frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j}}{C_{diss,i}^j + C_{DOC,i}^j} = \frac{\frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS}}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w} \right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2} \right) Sc_{w,i}^{-0.67} \left(3.15 x 10^{7} \right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2} \right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = \left(1.32 + 0.009 \bullet T_a\right) x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27053%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			33.13706%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.53471%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			6.15876%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00410%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.92923%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			79.43383%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			4.94622%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			53.83330%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			2.46695%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.98867%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.31
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.44
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	2,743.46
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}+K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}+K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}+K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed}+K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6}+K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	7.90	mg/L
Sbio_zoo,1	2.5		TSS_2	0.56	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	3.11E-01				
Sbio_dead,2	4.37E-01				
S_abio, sed	5.28E+04				
S_bio_dead,sed	2.74E+03				
S_sed,total	5.56E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

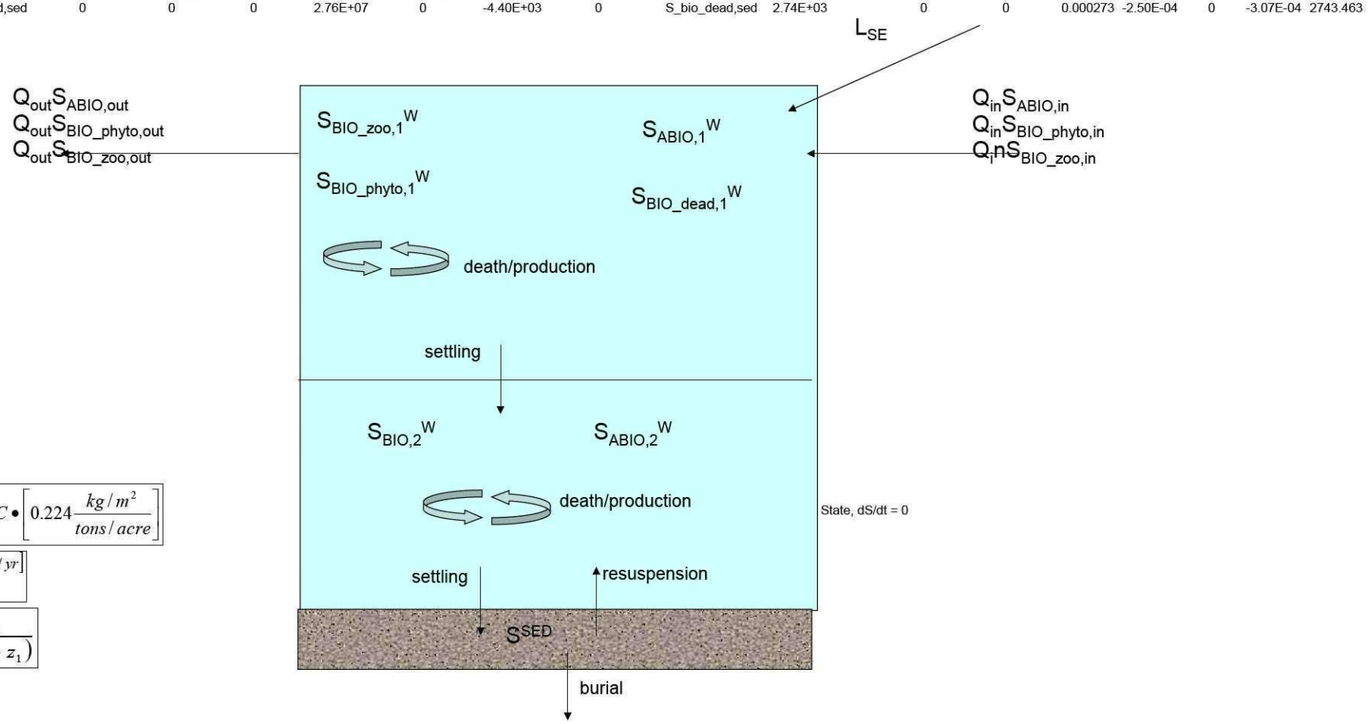
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	1.01E+07	S_bio_dead,1	3.11E-01	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.311342
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	4.37E-01	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.4367
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	2.74E+03	0	0	0.000273	-2.50E-04	0	-3.07E-04	2743.463



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	0.00000016	1	2
k_meth_2	abiotic* methylation in layer 2		per day	0.0000016	1	4
k_meth_1	abiotic methylation in layer 1		per yr	0.0000584		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000584		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00885	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.06871		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.04271		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.33137		
k_meth_1	abiotic methylation in layer 1		per yr	5.17E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	2.34E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	0.00000048	1	2
k_meth_b	biotic methylation in sediments		per yr	0.0001752		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	0.000000016	1
k_demeth_2	biotic demethylation in layer 2		per day	0.00000016	
k_demeth_1	biotic demethylation in layer 1		per yr	0.00000584	
k_demeth_2	biotic demethylation in layer 2		per yr	0.0000584	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.85E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			3.31E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	3.01E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	2.34E-05	

$$k_{demeth} = k_{demeth\_base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608. mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	0.00000096	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.0003504		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photorad\_i} = k_{photorad\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Belted Kingfisher – Varied Diet

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	48.90245623
MeHg	7.33E-08	g/m3	0.07332	75.12997546

Total Mercury Concentration in Contaminated Sediment, dry weight	40.7	ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio			
HgII	7,182,936	1	
MeHg	15,887	1	
Kd_bio			
HgII	17,941,378	1	
MeHg	2,581,565	1	
Kd_DOC			
HgII	301,427	1	
MeHg	310,000	1	
	PCT ERROR	CLEANUP	
MeHg Filtered	3.65	12.02	
HgT Filtered	-20.91		
MeHg Unfilter	-31.54		
HgT Unfiltere	244.41		

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.58	ng/L		-15.58	-100	0.47	ng/L	4.80	ng/L
	HgII Filtered	2.97	ng/L		-2.97	-100	0.10	ng/L	0.92	ng/L
	MeHg Filtered	0.74	ng/L	0.77	0.03	3.6500678	0.04	ng/L	0.24	ng/L
	HgT Filtered	19.29	ng/L	15.26	-4.03	-20.91065	0.61	ng/L	5.96	ng/L
	Hg0 Unfiltered	15.58	ng/L		-15.58	-100	0.47	ng/L	4.80	ng/L
	HgII Unfiltered	57.66	ng/L		-57.66	-100	1.87	ng/L	17.86	ng/L
	MeHg Unfiltered	4.06	ng/L	2.78	-1.28	-31.54439	0.21	ng/L	1.31	ng/L
	HgT Unfiltered	77.30	ng/L	266.23	188.93	244.4148	2.55	ng/L	23.97	ng/L
Hypolimnion	Hg0 Filtered	110.39	ng/L		-110.39	-100	1.43	ng/L	32.65	ng/L
	HgII Filtered	244.01	ng/L		-244.01	-100	3.08	ng/L	72.12	ng/L
	MeHg Filtered	10.76	ng/L		-10.76	-100	0.29	ng/L	3.29	ng/L
	HgT Filtered	365.17	ng/L		-365.17	-100	4.79	ng/L	108.06	ng/L
	Hg0 Unfiltered	110.39	ng/L		-110.39	-100	1.43	ng/L	32.65	ng/L
	HgII Unfiltered	609.90	ng/L		-609.90	-100	7.69	ng/L	180.25	ng/L
	MeHg Unfiltered	12.80	ng/L		-12.80	-100	0.34	ng/L	3.91	ng/L
	HgT Unfiltered	733.10	ng/L		-733.10	-100	9.46	ng/L	216.82	ng/L
Sediment										
	Hg0 porewater	110.39	ng/L		-110.39	-100	1.43	ng/L	32.654	ng/L
	HgII porewater	290.76	ng/L		-290.76	-100	3.60	ng/L	85.889	ng/L
	MeHg porewater	2.84	ng/L		-2.84	-100	0.06	ng/L	0.858	ng/L
	HgT porewater	403.99	ng/L		-403.99	-100	5.10	ng/L	119.400	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.65	ug/g		-40.65	-100	0.27	ug/g	12.01	ug/g
	MeHg bulk, dry	0.04611	ug/g	0.00658	-0.04	-85.72872	0.00	ug/g	0.01	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.505	ug/g	12.02	ug/g
Fish	Trophic Level 3	0.68	ug/g		-0.68	-100	0.035	ug/g	0.22	ug/g
	Trophic Level 4	1.48	ug/g		-1.48	-100	0.075	ug/g	0.48	ug/g
	HI	3.10					0.16		1.00	
	Sensitive Indicator	Kingfisher					Kingfisher		Kingfisher	
	Target C_sed, dry	12.02	ug/g	Note: 8						
	Target C_sed, wet	5.42	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.16E-07	per day	1.16E-04
	Hypolimnion	1.16E-06	per day	
	Sediment	3.49E-07	per day	
Demethylation	Epilimnion	1.16E-08	per day	
	Hypolimnion	1.16E-07	per day	
	Sediment	6.98E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

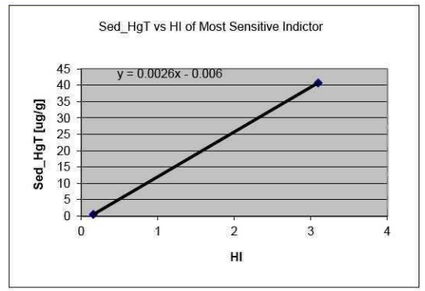
Human and Wildlife Exposure Risk Results

8,594

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.83	0.04	0.27
Otter	0.89	0.05	0.29
Mink	**1.74**	0.09	0.56
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	**1.59**	0.08	0.51
Kingfisher	**3.10**	0.16	**1.00**
Wood Duck	0.62	0.03	0.20
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
3.10	40.70
0.16	0.50
m =	13.681
b=	-1.658
Sed_HgT	12.023
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under tools. Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.74	0.04	0.240	ng/L

Biota

Trophic Level 1: Phytoplankton	0.14	0.01	0.05	ug Hg/ g wet weight
Trophic Level 2: Insects	0.12	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.13	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.68	0.03	0.22	ug Hg/ g wet weight
Trophic Level 4: Bass	1.48	0.08	0.48	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.80	0.04	0.26	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.14	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.13	0.01	0.04	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Wildlife Specific Parameters									Contaminated Sediment Calculations								
Animal	**Body Weight** [kg in wet weight]	**Ingestion Rate** [kg wet weight/d]	**Drinking rate** [L/d]	**Percent of Diet from Trophic Level 1 : Phytoplankton and Plants** --	**Percent of Diet from Trophic Level 2 : Insects** --	**Percent of Diet from Trophic Level 2 : Crayfish or Frogs** --	**Percent of Diet from Trophic Level 3 : Fish** --	**Percent of Diet from Trophic Level 4 : Fish** --	**Percent of Diet from nonaquatic sources** --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	62	0	0	0	62	75	0.83
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	2	50	15	67	75	0.89
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	6	5	119	130	75	**1.74**
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	30	11	55	0	95	60	**1.59**
Kingfisher	0.15	0.086	0.017	0%	0%	18%	23%	10%	50%	0	0	0	13	88	85	186	60	**3.10**
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	29	8	0	0	0	37	60	0.62
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	1	2	11	14	5000	0.00
Human	**Human Specific Parameters**																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.006	0.00	3.18	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.10	2.58	0.75	3	75	0.05
0.004	0.00	0.00	0.32	0.23	6.10	7	75	0.09
0.002	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.018	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.003	0.00	1.53	0.55	2.79	0.00	5	60	0.08
0.004	0.00	0.00	0.69	4.47	4.33	9	60	0.16
0.003	1.47	0.43	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.04	0.09	0.58	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.038	0.00	20.14	0.00	0.00	0.00	20	75	0.27
0.020	0.00	0.00	0.64	16.29	4.73	22	75	0.29
0.024	0.00	0.00	2.04	1.48	38.59	42	75	0.56
0.011	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.113	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.017	0.00	9.69	3.48	17.67	0.00	31	60	0.51
0.027	0.00	0.00	4.33	28.29	27.38	60	60	**1.00**
0.016	9.27	2.73	0.00	0.00	0.00	12	60	0.20
0.000	0.00	0.00	0.24	0.60	3.66	4	5000	0.00
							RfD	
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.005	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Belted Kingfisher – Varied Diet

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes			Oligo	Meso	Eutro	Dystro	
1	Trophic Status is determined DOC in Epiliminon as:		<3	3-5	5-10	10+	mg DOC/L
	from Wetzel	Flag	1	2	3	4	
2	Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)
HgII	mean	3.8	5.3	4.9	5.4
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6
	n	17	35	2	3
MeHg	mean	2.8	4.9	3.9	5
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5
	n	11	2		

Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
			199526.23				
630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	1584893.2	100000	316227.77	8	635462.6		12,679,146
			630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.74E-07	0.47
C_HgII_1_Aq			g/m3	9.64E-08	0.10
C_MeHg_1_Aq			g/m3	3.79E-08	0.04
C_Hg0_2_Aq			g/m3	1.43E-06	1.43
C_HgII_2_Aq			g/m3	3.08E-06	3.08
C_MeHg_2_Aq			g/m3	2.86E-07	0.29
C_Hg0_pore			g/m3	1.43E-06	1.43
C_HgII_pore			g/m3	3.60E-06	3.60
C_MeHg_pore			g/m3	6.35E-08	0.06
C_HgT_1_filtered			g/m3	6.08E-07	0.61
C_HgT_2_filtered			g/m3	4.79E-06	4.79
C_HgT_Sed_filtered			g/m3	5.10E-06	5.10
C_Hg0_1_T			g/m3	4.74E-07	0.47
C_HgII_1_T			g/m3	1.87E-06	1.87
C_MeHg_1_T			g/m3	2.07E-07	0.21
C_Hg0_2_T			g/m3	1.43E-06	1.43
C_HgII_2_T			g/m3	7.69E-06	7.69
C_MeHg_2_T			g/m3	3.40E-07	0.34
C_Hg0_sed, bulk			g/m3	1.19E-06	1
C_HgII_1_sed, bulk			g/m3	2.27E-01	226,907
C_MeHg_1_sed, bulk			g/m3	4.65E-04	465
C_Hg0_sed, wet			g/g	9.27E-13	0.000
C_HgII_1_sed, wet			g/g	2.72E-07	0.272
C_MeHg_1_sed, wet			g/g	4.22E-14	0.000
C_HgT_sed,wet			g/g	2.72E-07	0.272
C_Hg0_sed, dry weight			g/g	2.63E-12	0.0000
C_HgII_1_sed, dry weight			g/g	5.04E-07	0.5037
C_MeHg_1_sed, dry weight			g/g	1.03E-09	0.0010
C_HgT_1			g/m3	2.55E-06	2.551
C_HgT_2			g/m3	9.46E-06	9.457
C_HgT_Sed, dry weight			g/g	5.05E-07	0.505

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)	8.13%	73.29%	18.58%
Layer 2		3.60%	81.28%	15.12%
Sediments		0.20%	99.80%	0.00%

Q'	Bulk Exchange Flow	m3/yr	3,017,619
Qin	Inflow	m3/yr	3,474,314
Qout	Outflow	m3/yr	3,474,314
Aw	Surface Area of the Water Body	m2	378,381
E	Exchange rate	m2/yr	2
V_1	Volume of Layer 1	m3	183,741
V_2	Volume of Layer 2	m3	37,838
z1	depth of first water layer	m	0.49
z2	depth of second water layer	m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.009
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.031
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.069
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.141
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.043
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.152
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.331
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.700

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red,2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	4.740E-07	-1.21E-08	-1.12E-08	-5.13E-09	-1.14E-08	-1.13E-08	-5.60E-09	-1.14E-08	-1.13E-08	-5.60E-09	4.74001E-07
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.870E-06	-2.70E-08	-4.47E-08	-1.21E-08	-3.98E-08	-4.17E-08	-1.42E-08	-3.98E-08	-4.17E-08	-1.42E-08	1.86967E-06
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	2.074E-07	-7.21E-10	-1.15E-09	-1.60E-07	-2.55E-09	-2.83E-09	-1.48E-07	-2.55E-09	-2.88E-09	-1.48E-07	2.07388E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.430E-06	-2.197E-08	-3.407E-08	-1.369E-08	-1.17E-07	-8.15E-08	-2.15E-08	-1.17E-07	-8.14E-08	-2.15E-08	1.4299E-06
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	7.687E-06	-1.147E-07	-1.835E-07	-6.226E-08	-4.06E-07	-4.50E-07	-8.83E-08	-4.06E-07	-4.50E-07	-8.85E-08	7.68731E-06
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T	3.402E-07	-2.334E-09	-3.731E-09	-1.856E-07	-8.26E-09	-9.16E-09	-4.79E-07	-8.26E-09	-9.32E-09	-4.78E-07	3.40213E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	1.187E-06	-1.82E-08	-2.83E-08	-1.14E-08	-9.73E-08	-6.76E-08	-1.78E-08	-4.02E-06	-6.76E-08	-1.79E-08	1.18682E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.27E+08	0.00E+00	0.00E+00	-4.29E+03	2.89E+00	0.00E+00	C_HgII_1_sed	2.269E-01	-3.39E-03	-5.42E-03	-1.84E-03	-1.20E-02	-1.33E-02	-2.61E-03	-1.20E-02	-1.35E-02	-2.61E-03	0.226906529
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	4.648E-04	-3.80E-06	-6.08E-06	-2.13E-04	-1.35E-05	-1.49E-05	-5.48E-04	-1.35E-05	-1.52E-05	-7.79E-04	0.000464799

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.005
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.062
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.099
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.794
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.049
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.025
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.538
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.159
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		1.32E-05
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		1.13E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{zw} = \frac{E_{zw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \quad \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS} = \frac{}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C Hg0 1 Aq			g/m3	1.56E-05	15.58
C HgII 1 Aq			g/m3	2.97E-06	2.97
C MeHg 1 Aq			g/m3	7.43E-07	0.74
C Hg0 2 Aq			g/m3	1.10E-04	110.39
C HgII 2 Aq			g/m3	2.44E-04	244.01
C MeHg 2 Aq			g/m3	1.08E-05	10.76
C Hg0 pore			g/m3	1.10E-04	110.39
C HgII pore			g/m3	2.91E-04	290.76
C MeHg pore			g/m3	2.84E-06	2.84
C HgT 1 filtered			g/m3	1.93E-05	19.29
C HgT 2 filtered			g/m3	3.65E-04	365.17
C HgT Sed filtered			g/m3	4.04E-04	403.99
C Hg0 1 T			g/m3	1.56E-05	15.58
C HgII 1 T			g/m3	5.77E-05	57.66
C MeHg 1 T			g/m3	4.06E-06	4.06
C Hg0 2 T			g/m3	1.10E-04	110.39
C HgII 2 T			g/m3	6.10E-04	609.90
C MeHg 2 T			g/m3	1.28E-05	12.80
C Hg0 sed			g/m3	9.16E-05	91.63
C HgII 1 sed			g/m3	1.83E+01	18314487.35
C MeHg 1 sed			g/m3	2.08E-02	20771.02
C Hg0 sed, wet			g/g	3.46E-11	0.000
C HgII 1 sed, wet			g/g	1.43E-05	14.303
C MeHg 1 sed, wet			g/g	2.49E-08	0.025
C HgT sed,wet			g/g	1.43E-05	14.328
C Hg0 sed, dry weight			g/g	2.03E-10	0.00
C HgII 1 sed, dry weight			g/g	4.07E-05	40.65
C MeHg 1 sed, dry weight			g/g	4.61E-08	0.05
C HgT 1			g/m3	7.73E-05	77.30
C HgT 2			g/m3	7.33E-04	733.10
C HgT Sed			g/g	4.07E-05	40.70
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg T/Hg T)		5.25%	74.59%	20.15%
Layer 2			1.75%	83.19%	15.06%
Sediments			0.11%	99.89%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V 1	Volume of Layer 1	Aw*z 1	m3	183,741	
V 2	Volume of Layer 2	Aw*z 2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	
f aq Hg0 w 1	aqueous phase fraction of Hg0 in water column, layer 1				100.00000%
f aq HgII w 1	aqueous phase fraction of HgII in water column, layer 1				0.88548%
f aq MeHg w 1	aqueous phase fraction of MeHg in water column, layer 1				3.06930%
f aq Hg0 w 2	aqueous phase fraction of Hg0 in water column, layer 2				100.00000%
f aq HgII w 2	aqueous phase fraction of HgII in water column, layer 2				6.87088%
f aq MeHg w 2	aqueous phase fraction of MeHg in water column, layer 2				14.10566%
f DOC Hg0 w 1	DOC complexed fraction of Hg0 in water column, layer 1				0.00000%
f DOC Hg0 w 2	DOC complexed fraction of HgII in water column, layer 1				4.27053%
f DOC HgII w 1	DOC complexed fraction of MeHg in water column, layer 1				15.22372%
f DOC HgII w 2	DOC complexed fraction of Hg0 in water column, layer 2				0.00000%
f DOC MeHg w 1	DOC complexed fraction of HgII in water column, layer 2				33.13706%
f DOC MeHg w 2	DOC complexed fraction of MeHg in water column, layer 2				69.96409%
f abio Hg0 w 1	abiotic particulate phase fraction of Hg0 in water column, layer 1				0.00000%
f abio HgII w 1	abiotic particulate phase fraction of HgII in water column, layer 1				0.53471%
f abio MeHg w 1	abiotic particulate phase fraction of MeHg in water column, layer 1				0.00410%
f abio Hg0 w 2	abiotic particulate phase fraction of Hg0 in water column, layer 2				0.00000%
f abio HgII w 2	abiotic particulate phase fraction of HgII in water column, layer 2				6.15876%
f abio MeHg w 2	abiotic particulate phase fraction of MeHg in water column, layer 2				0.02796%

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in} C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in} C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in} C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot A_w \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{eq} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	1	2	3	4	5	6	7	8	9	b
C Hg0 1 T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01
C HgII 1 T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01
C MeHg 1 T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01
C Hg0 2 T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00
C HgII 2 T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00
C MeHg 2 T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00
C Hg0 sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00
C HgII 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01
C MeHg 1 sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00

Matrix	Solution	Inverted Matrix									x=b/A
C Hg0 1 T	1.558E-05	-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.34E-07	-2.77E-09	1.6E-05
C HgII 1 T	5.766E-05	-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.78E-09	5.8E-05
C MeHg 1 T	4.061E-06	-9.27E-17	-3.53E-16	-1.59E-07	7.27E-15	-4.95E-16	-1.47E-07	8.42E-13	2.13E-07	-1.47E-07	4.1E-06
C Hg0 2 T	1.104E-04	-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.51E-09	-4.51E-08	6.02E-06	-1.11E-09	0.00011
C HgII 2 T	6.099E-04	-1.979E-09	-3.165E-09	5.934E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.33E-05	2.43E-08	0.00061
C MeHg 2 T	1.280E-05	7.949E-17	-4.998E-16	-1.842E-07	2.36E-14	-1.59E-15	-4.76E-07	2.72E-12	6.88E-07	-4.76E-07	1.3E-05
C Hg0 sed	9.163E-05	-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.20E-10	9.2E-05
C HgII 1 sed	1.831E+01	1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.44E-04	3.95E-06	9.99E-01	7.75E-04	18.3145
C MeHg 1 sed	2.077E-02	5.27E-13	-1.69E-13	-2.10E-04	3.95E-11	-1.42E-12	-5.44E-04	4.44E-09	1.12E-03	-7.75E-04	0.02077

A*x=b

C T sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.98867%
L_T,Hg0	Total Load, Hg0		g/yr	3.99E-01
L_T,HgII	Total Load, HgII		g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg		g/yr	7.43E-01
Rate Constants				
kw_v,Hg0	water column volatilization loss rate constant, Hg0		per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII		per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg		per yr	0.65
kw_oxid_1	water column oxidation rate constant		per yr	610.22
kw_oxid_2	water column oxidation rate constant		per yr	525.60
kw_red_1	water column reduction rate constant, layer 2		per yr	246.95
kw_red_2	water column reduction rate constant, layer 2		per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1		per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2		per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1		per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2		per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1		per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2		per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant		per yr	0.00
kb_oxid	benthic oxidation rate constant		per yr	0.00
kb_red	benthic reduction rate constant		per yr	0.00
kb_methy	benthic methylation rate constant		per yr	0.00
kb_demeth	benthic demethylation rate constant		per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant		per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity		m/yr	4792.628412
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	7.90
TSS+2			mg/L	0.56
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_HgII_1	Effective K for Hg0 in layer 2		L/kg	2.33E+06
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.66E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	3.37E+05

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{soe}^{j} C_{soe,i}^{j}\right)}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS} = \frac{}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.80E-06	4.80
C_HgII_1_Aq			g/m3	9.21E-07	0.92
C_MeHg_1_Aq			g/m3	2.40E-07	0.24
C_Hg0_2_Aq			g/m3	3.27E-05	32.65
C_HgII_2_Aq			g/m3	7.21E-05	72.12
C_MeHg_2_Aq			g/m3	3.29E-06	3.29
C_Hg0_pore			g/m3	3.27E-05	32.65
C_HgII_pore			g/m3	8.59E-05	85.89
C_MeHg_pore			g/m3	8.58E-07	0.86
C_HgT_1_filtered			g/m3	5.96E-06	5.96
C_HgT_2_filtered			g/m3	1.08E-04	108.06
C_HgT_Sed_filtered			g/m3	1.19E-04	119.40
C_Hg0_1_T			g/m3	4.80E-06	4.80
C_HgII_1_T			g/m3	1.79E-05	17.86
C_MeHg_1_T			g/m3	1.31E-06	1.31
C_Hg0_2_T			g/m3	3.27E-05	32.65
C_HgII_2_T			g/m3	1.80E-04	180.25
C_MeHg_2_T			g/m3	3.91E-06	3.91
C_Hg0_sed			g/m3	2.71E-05	27.10
C_HgII_1_sed			g/m3	5.41E+00	5,409,978.52
C_MeHg_1_sed			g/m3	6.28E-03	6,283.63
C_Hg0_sed, wet			g/g	1.02E-11	0.00
C_HgII_1_sed, wet			g/g	4.22E-06	4.22
C_MeHg_1_sed, wet			g/g	7.52E-09	0.01
C_HgT_sed,wet			g/g	4.23E-06	4.23
C_Hg0_sed, dry weight			g/g	6.02E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.20E-05	12.01
C_MeHg_1_sed, dry weight			g/g	1.39E-08	0.01
C_HgT_1			g/m3	2.40E-05	23.97
C_HgT_2			g/m3	2.17E-04	216.82
C_HgT_Sed, dry weight			g/g	1.20E-05	12.02
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		5.47%	74.49%	20.03%
Layer 2			1.80%	83.14%	15.06%
Sediments			0.12%	99.88%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			4.27053%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			33.13706%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	4.802E-06	-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.34E-07	-2.77E-09	4.8E-06
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.786E-05	-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.78E-09	1.8E-05
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	1.312E-06	-9.27E-17	-3.53E-16	-1.59E-07	7.27E-15	-4.95E-16	-1.47E-07	8.42E-13	2.13E-07	-1.47E-07	1.3E-06
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	3.265E-05	-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.51E-09	-4.51E-08	6.02E-06	-1.11E-09	3.3E-05
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	1.803E-04	-1.979E-09	-3.165E-09	5.934E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.33E-05	2.43E-08	0.00018
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	4.31E+03	0.00E+00	0.00E+00	C_MeHg_2_T	3.912E-06	7.949E-17	-4.998E-16	-1.842E-07	2.36E-14	-1.59E-15	-4.76E-07	2.72E-12	6.88E-07	-4.76E-07	3.9E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	2.710E-05	-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.20E-10	2.7E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	5.42E+00	C_HgII_1_sed	5.410E+00	1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.44E-04	3.95E-06	9.99E-01	7.75E-04	5.40998
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	6.284E-03	5.27E-13	-1.69E-13	-2.10E-04	3.95E-11	-1.42E-12	-5.44E-04	4.44E-09	1.12E-03	-7.75E-04	0.00628

A*x=b

Target C_sed, wet 5.416289254 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	388.36
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	246.95
kw_red_2	water column reduction rate constant	per yr	107.40
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for	per yr	6.43
kw_mer	water column *mer* cleavage demeth	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

$$kw_{v,i} = \frac{K_{v,1} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS} = \frac{}{C_{diss,i}^j + C_{DOC,i}^j} \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = \left(1.32 + 0.009 \bullet T_a\right)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27053%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			33.13706%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.53471%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			6.15876%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00410%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.92923%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			79.43383%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			4.94622%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			53.83330%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			2.46695%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.98867%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.31
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.44
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	2,743.46
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	7.90	mg/L
Sbio_zoo,1	2.5		TSS_2	0.56	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	3.11E-01				
Sbio_dead,2	4.37E-01				
S_abio, sed	5.28E+04				
S_bio_dead,sed	2.74E+03				
S_sed,total	5.56E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

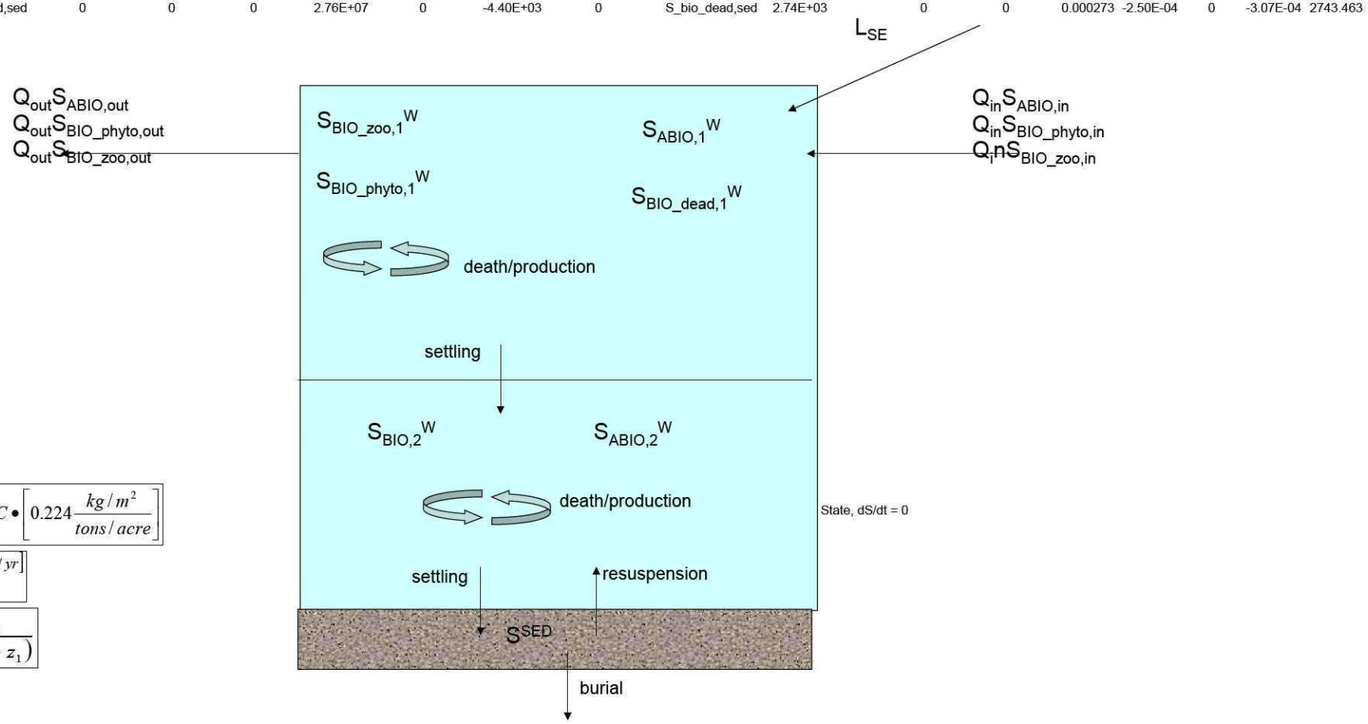
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	1.01E+07	S_bio_dead,1	3.11E-01	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.311342
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	4.37E-01	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.4367
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	2.74E+03	0	0	0.000273	-2.50E-04	0	-3.07E-04	2743.463



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00885	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.06871		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.04271		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.33137		
k_meth_1	abiotic methylation in layer 1		per yr	3.76E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.70E-05		

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

if anoxic:

$$k_{meth} = k_{meth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.85E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			3.31E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.19E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.70E-05	

$$k_{demeth} = k_{demeth,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	1
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

$$\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x}\,dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$$

$$z_2 = x_2 - x_1$$

$$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x}\,dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$$

$$\eta_{UV\text{-}B} = 0.4415 * (DOC)^{1.86}$$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43* ,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Belted Kingfisher

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	48.90245623
MeHg	7.33E-08	g/m3	0.07332	75.12997546

Total Mercury Concentration in Contaminated Sediment, dry weight	40.7 ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator	1

Kd_abio

HgII	7,182,936	1
MeHg	15,887	1

Kd_bio

HgII	17,941,378	1
MeHg	2,581,565	1

Kd_DOC

HgII	301,427	1
MeHg	310,000	1

	PCT ERROR	CLEANUP
MeHg Filtered	3.65	4.87
HgT Filtered	-20.91	
MeHg Unfilter	-31.54	
HgT Unfiltere	244.41	

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.58	ng/L		-15.58	-100	0.47	ng/L	2.11	ng/L
	HgII Filtered	2.97	ng/L		-2.97	-100	0.10	ng/L	0.41	ng/L
	MeHg Filtered	0.74	ng/L	0.77	0.03	3.6500678	0.04	ng/L	0.11	ng/L
	HgT Filtered	19.29	ng/L	15.26	-4.03	-20.91065	0.61	ng/L	2.64	ng/L
	Hg0 Unfiltered	15.58	ng/L		-15.58	-100	0.47	ng/L	2.11	ng/L
	HgII Unfiltered	57.66	ng/L		-57.66	-100	1.87	ng/L	7.93	ng/L
	MeHg Unfiltered	4.06	ng/L	2.78	-1.28	-31.54439	0.21	ng/L	0.63	ng/L
	HgT Unfiltered	77.30	ng/L	266.23	188.93	244.4148	2.55	ng/L	10.67	ng/L
Hypolimnion	Hg0 Filtered	110.39	ng/L		-110.39	-100	1.43	ng/L	13.26	ng/L
	HgII Filtered	244.01	ng/L		-244.01	-100	3.08	ng/L	29.24	ng/L
	MeHg Filtered	10.76	ng/L		-10.76	-100	0.29	ng/L	1.42	ng/L
	HgT Filtered	365.17	ng/L		-365.17	-100	4.79	ng/L	43.93	ng/L
	Hg0 Unfiltered	110.39	ng/L		-110.39	-100	1.43	ng/L	13.26	ng/L
	HgII Unfiltered	609.90	ng/L		-609.90	-100	7.69	ng/L	73.09	ng/L
	MeHg Unfiltered	12.80	ng/L		-12.80	-100	0.34	ng/L	1.69	ng/L
	HgT Unfiltered	733.10	ng/L		-733.10	-100	9.46	ng/L	88.05	ng/L
Sediment										
	Hg0 porewater	110.39	ng/L		-110.39	-100	1.43	ng/L	13.264	ng/L
	HgII porewater	290.76	ng/L		-290.76	-100	3.60	ng/L	34.789	ng/L
	MeHg porewater	2.84	ng/L		-2.84	-100	0.06	ng/L	0.365	ng/L
	HgT porewater	403.99	ng/L		-403.99	-100	5.10	ng/L	48.417	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.65	ug/g		-40.65	-100	0.27	ug/g	4.86	ug/g
	MeHg bulk, dry	0.04611	ug/g	0.00658	-0.04	-85.72872	0.00	ug/g	0.01	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.505	ug/g	4.87	ug/g
Fish	Trophic Level 3	0.68	ug/g		-0.68	-100	0.035	ug/g	0.10	ug/g
	Trophic Level 4	1.48	ug/g		-1.48	-100	0.075	ug/g	0.23	ug/g
	HI	6.49					0.33		1.00	
	Sensitive Indicator	Kingfisher					Kingfisher		Kingfisher	
	Target C_sed, dry	4.87	ug/g	Note: 8						
	Target C_sed, wet	2.19	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.16E-07	per day	1.16E-04
	Hypolimnion	1.16E-06	per day	
	Sediment	3.49E-07	per day	
Demethylation	Epilimnion	1.16E-08	per day	
	Hypolimnion	1.16E-07	per day	
	Sediment	6.98E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

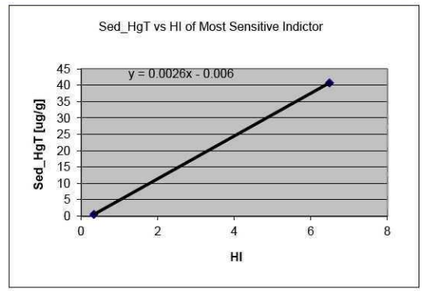
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.83	0.04	0.13
Otter	0.89	0.05	0.14
Mink	**1.74**	0.09	0.27
Great Blue Heron	**3.38**	0.17	0.52
Little Blue Heron	**3.89**	0.20	0.60
Pied-bill Grebe	**1.59**	0.08	0.25
Kingfisher	**6.49**	0.33	**1.00**
Wood Duck	0.62	0.03	0.10
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
6.49	40.70
0.33	0.50
m =	6.529
b=	-1.658
Sed_HgT	4.870
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under tools. Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.74	0.04	0.114	ng/L

Biota

Trophic Level 1: Phytoplankton	0.14	0.01	0.02	ug Hg/ g wet weight
Trophic Level 2: Insects	0.12	0.01	0.02	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.13	0.01	0.02	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.68	0.03	0.10	ug Hg/ g wet weight
Trophic Level 4: Bass	1.48	0.08	0.23	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.80	0.04	0.12	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.14	0.01	0.02	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.13	0.01	0.02	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife

	Wildlife Specific Parameters									Contaminated Sediment Calculations								
Animal	**Body Weight** [kg in wet weight]	**Ingestion Rate** [kg wet weight/d]	**Drinking rate** [L/d]	**Percent of Diet from Trophic Level 1 : Phytoplankton and Plants** --	**Percent of Diet from Trophic Level 2 : Insects** --	**Percent of Diet from Trophic Level 2 : Crayfish or Frogs** --	**Percent of Diet from Trophic Level 3 : Fish** --	**Percent of Diet from Trophic Level 4 : Fish** --	**Percent of Diet from nonaquatic sources** --	Potential Dose from Water [ng/d/kg]	Potential Dose from Trophic Level 1 ug Hg / kg wet weight / d	Potential Dose from Trophic Level 2: Insects ug Hg/kg wet weight/d	Potential Dose from Trophic Level 2: Crayfish ug Hg/kg wet weight/d	Potential Dose from Trophic Level 3 ug Hg/kg wet weight/d	Potential Dose from Trophic Level 4 ug Hg/kg wet weight/d	Total Potential Dose ug Hg/kg wet weight/d	TRV ug Hg/kg wet weight/d	HQ (Total Dose / TRV) --
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	62	0	0	0	62	75	0.83
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	2	50	15	67	75	0.89
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	6	5	119	130	75	**1.74**
Great Blue Heron	2.2	0.509	0.1	0%	5%	10%	50%	35%	0%	0	0	1	3	79	120	203	60	**3.38**
Little Blue Heron	0.34	0.147	0.16	0%	25%	0%	75%	0%	0%	0	0	13	0	220	0	234	60	**3.89**
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	30	11	55	0	95	60	**1.59**
Kingfisher	0.15	0.086	0.017	0%	0%	0%	100%	0%	0%	0	0	0	0	389	0	389	60	**6.49**
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	29	8	0	0	0	37	60	0.62
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	1	2	11	14	5000	0.00
Human	**Human Specific Parameters**																RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.006	0.00	3.18	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.10	2.58	0.75	3	75	0.05
0.004	0.00	0.00	0.32	0.23	6.10	7	75	0.09
0.002	0.00	0.07	0.16	4.01	6.11	10	60	0.17
0.018	0.00	0.68	0.00	11.24	0.00	12	60	0.20
0.003	0.00	1.53	0.55	2.79	0.00	5	60	0.08
0.004	0.00	0.00	0.00	19.88	0.00	20	60	0.33
0.003	1.47	0.43	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.04	0.09	0.58	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.018	0.00	9.61	0.00	0.00	0.00	10	75	0.13
0.010	0.00	0.00	0.31	7.77	2.26	10	75	0.14
0.011	0.00	0.00	0.97	0.70	18.42	20	75	0.27
0.005	0.00	0.22	0.48	12.11	18.45	31	60	0.52
0.054	0.00	2.07	0.00	33.93	0.00	36	60	0.60
0.008	0.00	4.62	1.66	8.43	0.00	15	60	0.25
0.013	0.00	0.00	0.00	60.00	0.00	60	60	**1.00**
0.008	4.42	1.30	0.00	0.00	0.00	6	60	0.10
0.000	0.00	0.00	0.12	0.28	1.75	2	5000	0.00
							RfD	
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.002	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes							
	1 Trophic Status is determined DOC in Epiliminon as:		Oligo	Meso	Eutro	Dystro	
	from Wetzel	Flag	<3	3-5	5-10	10+	mg DOC/L
			1	2	3	4	
	2 Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893.2	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.38

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.74E-07	0.47
C_HgII_1_Aq			g/m3	9.64E-08	0.10
C_MeHg_1_Aq			g/m3	3.79E-08	0.04
C_Hg0_2_Aq			g/m3	1.43E-06	1.43
C_HgII_2_Aq			g/m3	3.08E-06	3.08
C_MeHg_2_Aq			g/m3	2.86E-07	0.29
C_Hg0_pore			g/m3	1.43E-06	1.43
C_HgII_pore			g/m3	3.60E-06	3.60
C_MeHg_pore			g/m3	6.35E-08	0.06
C_HgT_1_filtered			g/m3	6.08E-07	0.61
C_HgT_2_filtered			g/m3	4.79E-06	4.79
C_HgT_Sed_filtered			g/m3	5.10E-06	5.10
C_Hg0_1_T			g/m3	4.74E-07	0.47
C_HgII_1_T			g/m3	1.87E-06	1.87
C_MeHg_1_T			g/m3	2.07E-07	0.21
C_Hg0_2_T			g/m3	1.43E-06	1.43
C_HgII_2_T			g/m3	7.69E-06	7.69
C_MeHg_2_T			g/m3	3.40E-07	0.34
C_Hg0_sed, bulk			g/m3	1.19E-06	1
C_HgII_1_sed, bulk			g/m3	2.27E-01	226,907
C_MeHg_1_sed, bulk			g/m3	4.65E-04	465
C_Hg0_sed, wet			g/g	9.27E-13	0.000
C_HgII_1_sed, wet			g/g	2.72E-07	0.272
C_MeHg_1_sed, wet			g/g	4.22E-14	0.000
C_HgT_sed,wet			g/g	2.72E-07	0.272
C_Hg0_sed, dry weight			g/g	2.63E-12	0.0000
C_HgII_1_sed, dry weight			g/g	5.04E-07	0.5037
C_MeHg_1_sed, dry weight			g/g	1.03E-09	0.0010
C_HgT_1			g/m3	2.55E-06	2.551
C_HgT_2			g/m3	9.46E-06	9.457
C_HgT_Sed, dry weight			g/g	5.05E-07	0.505

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)	8.13%	73.29%	18.58%
Layer 2		3.60%	81.28%	15.12%
Sediments		0.20%	99.80%	0.00%

Q'	Bulk Exchange Flow		m3/yr	3,017,619
Qin	Inflow		m3/yr	3,474,314
Qout	Outflow		m3/yr	3,474,314
Aw	Surface Area of the Water Body		m2	378,381
E	Exchange rate		m2/yr	2
V_1	Volume of Layer 1	Aw*z_1	m3	183,741
V_2	Volume of Layer 2	Aw*z_2	m3	37,838
z1	depth of first water layer		m	0.49
z2	depth of second water layer		m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.009
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.031
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.069
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.141
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.043
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.152
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.331
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.700

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored1} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{2B} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{s1} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red1} \cdot V_w - kw_{met1} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{2B} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{met1} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{2B} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{2B} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{met1} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{2B} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{2B} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{2B} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{2B} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{met}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{2B} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	4.740E-07	-1.21E-08	-1.12E-08	-5.13E-09	-1.14E-08	-1.13E-08	-5.60E-09	-1.14E-08	-1.13E-08	-5.60E-09	4.74001E-07
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.870E-06	-2.70E-08	-4.47E-08	-1.21E-08	-3.98E-08	-4.17E-08	-1.42E-08	-3.98E-08	-4.17E-08	-1.42E-08	1.86967E-06
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	2.074E-07	-7.21E-10	-1.15E-09	-1.60E-07	-2.55E-09	-2.83E-09	-1.48E-07	-2.55E-09	-2.88E-09	-1.48E-07	2.07388E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.430E-06	-2.197E-08	-3.407E-08	-1.369E-08	-1.17E-07	-8.15E-08	-2.15E-08	-1.17E-07	-8.14E-08	-2.15E-08	1.4299E-06
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	7.687E-06	-1.147E-07	-1.835E-07	-6.226E-08	-4.06E-07	-4.50E-07	-8.83E-08	-4.06E-07	-4.50E-07	-8.85E-08	7.68731E-06
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T	3.402E-07	-2.334E-09	-3.731E-09	-1.856E-07	-8.26E-09	-9.16E-09	-4.79E-07	-8.26E-09	-9.32E-09	-4.78E-07	3.40213E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	1.187E-06	-1.82E-08	-2.83E-08	-1.14E-08	-9.73E-08	-6.76E-08	-1.78E-08	-4.02E-06	-6.76E-08	-1.79E-08	1.18682E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.27E+08	0.00E+00	0.00E+00	-4.29E+03	2.89E+00	0.00E+00	C_HgII_1_sed	2.269E-01	-3.39E-03	-5.42E-03	-1.84E-03	-1.20E-02	-1.33E-02	-2.61E-03	-1.20E-02	-1.35E-02	-2.61E-03	0.226906529
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	4.648E-04	-3.80E-06	-6.08E-06	-2.13E-04	-1.35E-05	-1.49E-05	-5.48E-04	-1.35E-05	-1.52E-05	-7.79E-04	0.000464799

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.005
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.062
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.099
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.794
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.049
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.025
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.538
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.159
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		1.32E-05
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		1.13E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{d}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}}}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.58
C_HgII_1_Aq			g/m3	2.97E-06	2.97
C_MeHg_1_Aq			g/m3	7.43E-07	0.74
C_Hg0_2_Aq			g/m3	1.10E-04	110.39
C_HgII_2_Aq			g/m3	2.44E-04	244.01
C_MeHg_2_Aq			g/m3	1.08E-05	10.76
C_Hg0_pore			g/m3	1.10E-04	110.39
C_HgII_pore			g/m3	2.91E-04	290.76
C_MeHg_pore			g/m3	2.84E-06	2.84
C_HgT_1_filtered			g/m3	1.93E-05	19.29
C_HgT_2_filtered			g/m3	3.65E-04	365.17
C_HgT_Sed_filtered			g/m3	4.04E-04	403.99
C_Hg0_1_T			g/m3	1.56E-05	15.58
C_HgII_1_T			g/m3	5.77E-05	57.66
C_MeHg_1_T			g/m3	4.06E-06	4.06
C_Hg0_2_T			g/m3	1.10E-04	110.39
C_HgII_2_T			g/m3	6.10E-04	609.90
C_MeHg_2_T			g/m3	1.28E-05	12.80
C_Hg0_sed			g/m3	9.16E-05	91.63
C_HgII_1_sed			g/m3	1.83E+01	18314487.35
C_MeHg_1_sed			g/m3	2.08E-02	20771.02
C_Hg0_sed, wet			g/g	3.46E-11	0.000
C_HgII_1_sed, wet			g/g	1.43E-05	14.303
C_MeHg_1_sed, wet			g/g	2.49E-08	0.025
C_HgT_sed,wet			g/g	1.43E-05	14.328
C_Hg0_sed, dry weight			g/g	2.03E-10	0.00
C_HgII_1_sed, dry weight			g/g	4.07E-05	40.65
C_MeHg_1_sed, dry weight			g/g	4.61E-08	0.05
C_HgT_1			g/m3	7.73E-05	77.30
C_HgT_2			g/m3	7.33E-04	733.10
C_HgT_Sed			g/g	4.07E-05	40.70
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		5.25%	74.59%	20.15%
Layer 2			1.75%	83.19%	15.06%
Sediments			0.11%	99.89%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.88548%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	3.06930%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	6.87088%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	4.27053%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	15.22372%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	33.13706%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.02796%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} \cdot V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{methR} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{methR} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg,2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{methR} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{methR} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg,2} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w}{\theta_{sed}}\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	1.558E-05
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	5.766E-05
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	4.061E-06
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.104E-04
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	6.099E-04
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T	1.280E-05
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	9.163E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed	1.831E+01
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	2.077E-02

Inverted Matrix

-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.34E-07	-2.77E-09	1.56E-05
-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.78E-09	5.77E-05
-9.27E-17	-3.53E-16	-1.59E-07	7.27E-15	-4.95E-16	-1.47E-07	8.42E-13	2.13E-07	-1.47E-07	4.06E-06
-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.51E-09	-4.51E-08	6.02E-06	-1.11E-09	0.00011
-1.979E-09	-3.165E-09	5.934E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.33E-05	2.43E-08	0.00061
7.949E-17	-4.998E-16	-1.842E-07	2.36E-14	-1.59E-15	-4.76E-07	2.72E-12	6.88E-07	-4.76E-07	1.28E-05
-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.20E-10	9.16E-05
1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.44E-04	3.95E-06	9.99E-01	7.75E-04	18.31449
5.27E-13	-1.69E-13	-2.10E-04	3.95E-11	-1.42E-12	-5.44E-04	4.44E-09	1.12E-03	-7.75E-04	0.020771

x=b/A

A*x=b

C_T_sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed} \cdot 3.1536 \text{x} 10^7}{z_{sed}}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	7.90
TSS+2			mg/L	0.56
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_Hg0_1	Effective K for Hg0 in layer 2		L/kg	2.33E+06
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.66E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	3.37E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{sed}^{j}C_{sed,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{sed}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	2.11E-06	2.11
C_HgII_1_Aq			g/m3	4.09E-07	0.41
C_MeHg_1_Aq			g/m3	1.14E-07	0.11
C_Hg0_2_Aq			g/m3	1.33E-05	13.26
C_HgII_2_Aq			g/m3	2.92E-05	29.24
C_MeHg_2_Aq			g/m3	1.42E-06	1.42
C_Hg0_pore			g/m3	1.33E-05	13.26
C_HgII_pore			g/m3	3.48E-05	34.79
C_MeHg_pore			g/m3	3.65E-07	0.36
C_HgT_1_filtered			g/m3	2.64E-06	2.64
C_HgT_2_filtered			g/m3	4.39E-05	43.93
C_HgT_Sed_filtered			g/m3	4.84E-05	48.42
C_Hg0_1_T			g/m3	2.11E-06	2.11
C_HgII_1_T			g/m3	7.93E-06	7.93
C_MeHg_1_T			g/m3	6.26E-07	0.63
C_Hg0_2_T			g/m3	1.33E-05	13.26
C_HgII_2_T			g/m3	7.31E-05	73.09
C_MeHg_2_T			g/m3	1.69E-06	1.69
C_Hg0_sed			g/m3	1.10E-05	11.01
C_HgII_1_sed			g/m3	2.19E+00	2,191,300.87
C_MeHg_1_sed			g/m3	2.67E-03	2,670.15
C_Hg0_sed, wet			g/g	4.15E-12	0.00
C_HgII_1_sed, wet			g/g	1.71E-06	1.71
C_MeHg_1_sed, wet			g/g	3.20E-09	0.00
C_HgT_sed,wet			g/g	1.71E-06	1.71
C_Hg0_sed, dry weight			g/g	2.44E-11	0.00
C_HgII_1_sed, dry weight			g/g	4.86E-06	4.86
C_MeHg_1_sed, dry weight			g/g	5.93E-09	0.01
C_HgT_1			g/m3	1.07E-05	10.67
C_HgT_2			g/m3	8.80E-05	88.05
C_HgT_Sed, dry weight			g/g	4.87E-06	4.87
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		5.87%	74.31%	19.82%
Layer 2			1.92%	83.01%	15.06%
Sediments			0.12%	99.88%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			4.27053%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			33.13706%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%	

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{sA} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{sA} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} \cdot V_w - v_{sA} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{sA} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{sA} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{sA} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	2.114E-06	-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.34E-07	-2.77E-09	2.1E-06
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	7.929E-06	-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.78E-09	7.9E-06
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	6.259E-07	-9.27E-17	-3.53E-16	-1.59E-07	7.27E-15	-4.95E-16	-1.47E-07	8.42E-13	2.13E-07	-1.47E-07	6.3E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.326E-05	-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.51E-09	-4.51E-08	6.02E-06	-1.11E-09	1.3E-05
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	7.309E-05	-1.979E-09	-3.165E-09	5.934E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.33E-05	2.43E-08	7.3E-05
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T	1.694E-06	7.949E-17	-4.998E-16	-1.842E-07	2.36E-14	-1.59E-15	-4.76E-07	2.72E-12	6.88E-07	-4.76E-07	1.7E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	1.101E-05	-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.20E-10	1.1E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	2.19E+00	C_HgII_1_sed	2.191E+00	1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.44E-04	3.95E-06	9.99E-01	7.75E-04	2.1913
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	2.670E-03	5.27E-13	-1.69E-13	-2.10E-04	3.95E-11	-1.42E-12	-5.44E-04	4.44E-09	1.12E-03	-7.75E-04	0.00267

A*x=b

Target C_sed, wet 2.193982028 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01

Rate Constants

kw_v,Hg0	water column volatilization loss rate c	per yr	388.36
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	246.95
kw_red_2	water column reduction rate constant	per yr	107.40
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for	per yr	6.43
kw_mer	water column *mer* cleavage demeth	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00

v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56

Effective Partition Coefficients for each Hg species and layer

K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

$$kw_{v,i} = \frac{K_{v,1} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536x10^7$$

$$K_{eff,i}^j = \frac{\frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j}}{C_{diss,i}^j + C_{DOC,i}^j} = \frac{\frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS}}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{w,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2}\right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = \left(1.32 + 0.009 \bullet T_a\right)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27053%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			33.13706%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.53471%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			6.15876%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00410%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.92923%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			79.43383%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			4.94622%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			53.83330%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			2.46695%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.98867%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.31
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.44
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	2,743.46
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}+K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}+K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}+K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed}+K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6}+K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	7.90	mg/L
Sbio_zoo,1	2.5		TSS_2	0.56	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	3.11E-01				
Sbio_dead,2	4.37E-01				
S_abio, sed	5.28E+04				
S_bio_dead,sed	2.74E+03				
S_sed,total	5.56E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

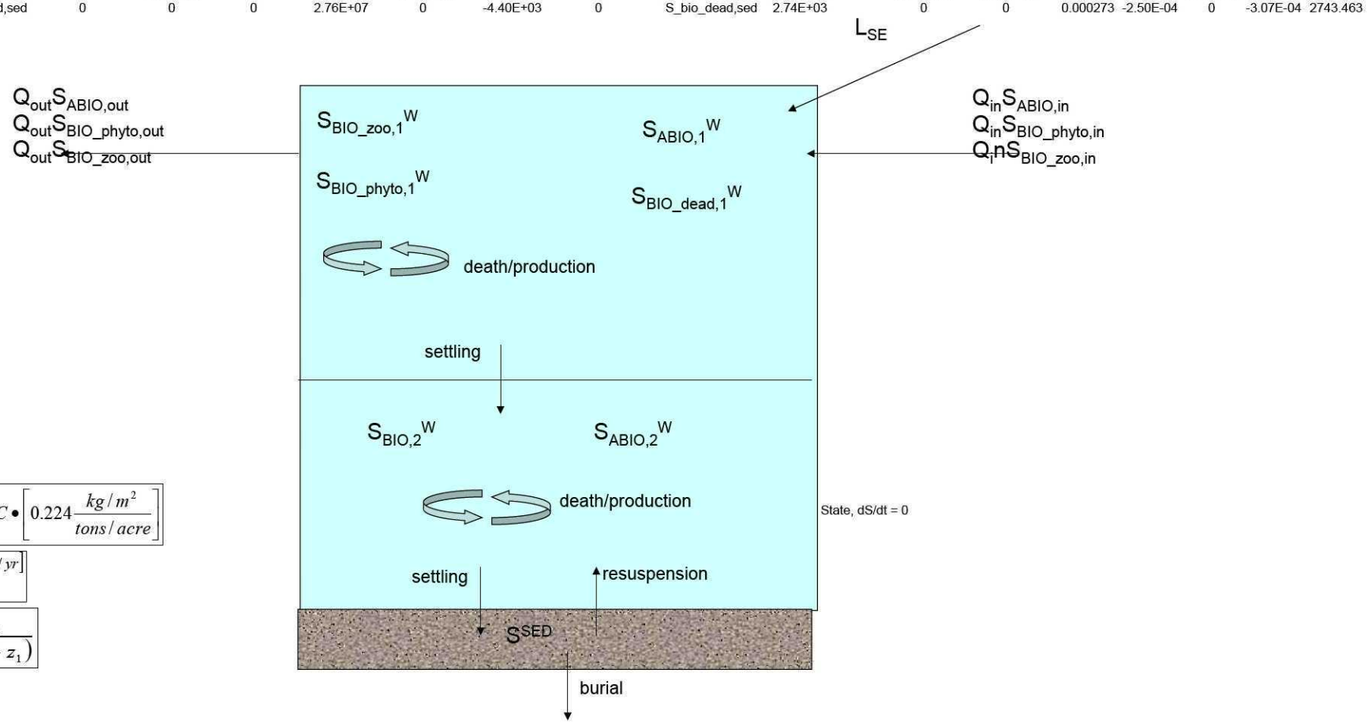
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix		Matrix Inversion						x=b/A
	1	2	3	4	5	6	b									
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	1.01E+07	S_bio_dead,1	3.11E-01	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.311342
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	4.37E-01	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.4367
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	2.74E+03	0	0	0.000273	-2.50E-04	0	-3.07E-04	2743.463



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00885	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.06871		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.04271		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.33137		
k_meth_1	abiotic methylation in layer 1		per yr	3.76E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.70E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.85E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			3.31E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.19E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.70E-05	

$$k_{demeth} = k_{demeth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{1.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location	
East	YES
West	NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Little Blue Heron

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3			
HgII	5.64E-06	g/m3	5.64	48.90245623	
MeHg	7.33E-08	g/m3	0.07332	75.12997546	Fish
Total Mercury Concentration in Contaminated Sediment, dry weight	40.7	ug/g			

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3	7
Cs,HgII	1.129080624	g/m3	
Cs,MeHg	4.13E-03	g/m3	

Required Hazard Index for Sensitive Indicator: 1

Kd_abio		
HgII	7,182,936	1
MeHg	15,887	1
Kd_bio		
HgII	17,941,378	1
MeHg	2,581,565	1
Kd_DOC		
HgII	301,427	1
MeHg	310,000	1
	PCT ERROR	CLEANUP
MeHg Filtered	3.65	9.22
HgT Filtered	-20.91	
MeHg Unfilte	-31.54	
HgT Unfiltere	244.41	

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.58	ng/L		-15.58	-100	0.47	ng/L	3.75	ng/L
	HgII Filtered	2.97	ng/L		-2.97	-100	0.10	ng/L	0.72	ng/L
	MeHg Filtered	0.74	ng/L	0.77	0.03	3.6500678	0.04	ng/L	0.19	ng/L
	HgT Filtered	19.29	ng/L	15.26	-4.03	-20.91065	0.61	ng/L	4.66	ng/L
	Hg0 Unfiltered	15.58	ng/L		-15.58	-100	0.47	ng/L	3.75	ng/L
	HgII Unfiltered	57.66	ng/L		-57.66	-100	1.87	ng/L	13.97	ng/L
	MeHg Unfiltered	4.06	ng/L	2.78	-1.28	-31.54439	0.21	ng/L	1.04	ng/L
	HgT Unfiltered	77.30	ng/L	266.23	188.93	244.4148	2.55	ng/L	18.76	ng/L
Hypolimnion	Hg0 Filtered	110.39	ng/L		-110.39	-100	1.43	ng/L	25.06	ng/L
	HgII Filtered	244.01	ng/L		-244.01	-100	3.08	ng/L	55.33	ng/L
	MeHg Filtered	10.76	ng/L		-10.76	-100	0.29	ng/L	2.56	ng/L
	HgT Filtered	365.17	ng/L		-365.17	-100	4.79	ng/L	82.95	ng/L
	Hg0 Unfiltered	110.39	ng/L		-110.39	-100	1.43	ng/L	25.06	ng/L
	HgII Unfiltered	609.90	ng/L		-609.90	-100	7.69	ng/L	138.29	ng/L
	MeHg Unfiltered	12.80	ng/L		-12.80	-100	0.34	ng/L	3.04	ng/L
	HgT Unfiltered	733.10	ng/L		-733.10	-100	9.46	ng/L	166.40	ng/L
	Sediment									
	Hg0 porewater	110.39	ng/L		-110.39	-100	1.43	ng/L	25.061	ng/L
	HgII porewater	290.76	ng/L		-290.76	-100	3.60	ng/L	65.879	ng/L
	MeHg porewater	2.84	ng/L		-2.84	-100	0.06	ng/L	0.665	ng/L
	HgT porewater	403.99	ng/L		-403.99	-100	5.10	ng/L	91.605	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.65	ug/g		-40.65	-100	0.27	ug/g	9.21	ug/g
	MeHg bulk, dry	0.04611	ug/g	0.00658	-0.04	-85.72872	0.00	ug/g	0.01	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.505	ug/g	9.22	ug/g
	Trophic Level 3	0.68	ug/g		-0.68	-100	0.035	ug/g	0.17	ug/g
	Trophic Level 4	1.48	ug/g		-1.48	-100	0.075	ug/g	0.38	ug/g
	HI	3.89					0.20		1.00	
	Sensitive Indicator	Little Blue Heron					Little Blue Heron		Little Blue Heron	
	Target C_sed, dry	9.22	ug/g	Note: 8						
	Target C_sed, wet	4.15	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.16E-07	per day	1.16E-04
	Hypolimnion	1.16E-06	per day	
	Sediment	3.49E-07	per day	
Demethylation	Epilimnion	1.16E-08	per day	
	Hypolimnion	1.16E-07	per day	
	Sediment	6.98E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

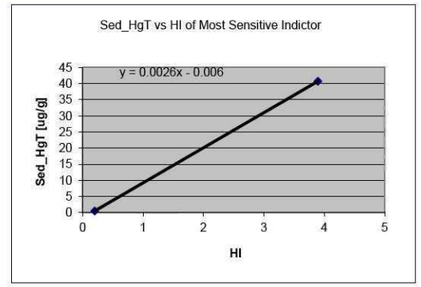
Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

Human and Wildlife Exposure Risk Results

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	0.83	0.04	0.21
Otter	0.89	0.05	0.23
Mink	**1.74**	0.09	0.45
Great Blue Heron	**3.38**	0.17	0.87
Little Blue Heron	**3.89**	0.20	**1.00**
Pied-bill Grebe	**1.59**	0.08	0.41
Kingfisher	0.00	0.00	0.00
Wood Duck	0.62	0.03	0.16
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
3.89	40.70
0.20	0.50
m =	10.880
b=	-1.658
Sed_HgT	9.222
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity. An exact result can be found by using the "Goal Seek" function under tools. Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

Site-Specific User Input	Required
Model Calculated	No input required
Data Necessary for certain sites	Only necessary if applicable to site of interest
Scenario 1 Output	
Scenario 2 Output	
Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	0.74	0.04	0.191	ng/L

Biota

Trophic Level 1: Phytoplankton	0.14	0.01	0.04	ug Hg/ g wet weight
Trophic Level 2: Insects	0.12	0.01	0.03	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.13	0.01	0.03	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.68	0.03	0.17	ug Hg/ g wet weight
Trophic Level 4: Bass	1.48	0.08	0.38	ug Hg/ g wet weight
Trophic Level 3: Silverside	0.80	0.04	0.21	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.14	0.01	0.04	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.13	0.01	0.03	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Body Weight	Ingestion Rate	Drinking rate	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants	Percent of Diet from Trophic Level 2 : Insects	Percent of Diet from Trophic Level 2 : Crayfish or Frogs	Percent of Diet from Trophic Level 3 : Fish	Percent of Diet from Trophic Level 4 : Fish	Percent of Diet from nonaquatic sources	Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Insects	Potential Dose from Trophic Level 2: Crayfish	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
Animal	[kg in wet weight]	[kg wet weight/d]	[L/d]	--	--	--	--	--	--	[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	62	0	0	0	62	75	0.83
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	2	50	15	67	75	0.89
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	6	5	119	130	75	**1.74**
Great Blue Heron	2.2	0.509	0.1	0%	5%	10%	50%	35%	0%	0	0	1	3	79	120	203	60	**3.38**
Little Blue Heron	0.34	0.147	0.16	0%	25%	0%	75%	0%	0%	0	0	13	0	220	0	234	60	**3.89**
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	30	11	55	0	95	60	**1.59**
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	29	8	0	0	0	37	60	0.62
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	1	2	11	14	5000	0.00
Human																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Wildlife Specific Parameters | **Contaminated Sediment Calculations** | **Human Specific Parameters**

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.006	0.00	3.18	0.00	0.00	0.00	3	75	0.04
0.003	0.00	0.00	0.10	2.58	0.75	3	75	0.05
0.004	0.00	0.00	0.32	0.23	6.10	7	75	0.09
0.002	0.00	0.07	0.16	4.01	6.11	10	60	0.17
0.018	0.00	0.68	0.00	11.24	0.00	12	60	0.20
0.003	0.00	1.53	0.55	2.79	0.00	5	60	0.08
0.004	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.003	1.47	0.43	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.04	0.09	0.58	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.031	0.00	16.02	0.00	0.00	0.00	16	75	0.21
0.016	0.00	0.00	0.51	12.96	3.76	17	75	0.23
0.019	0.00	0.00	1.62	1.17	30.69	33	75	0.45
0.009	0.00	0.37	0.79	20.18	30.75	52	60	0.87
0.090	0.00	3.44	0.00	56.56	0.00	60	60	**1.00**
0.014	0.00	7.70	2.77	14.05	0.00	25	60	0.41
0.022	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.013	7.37	2.17	0.00	0.00	0.00	10	60	0.16
0.000	0.00	0.00	0.19	0.47	2.91	4	5000	0.00
							RfD	
0.003	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.004	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Little Blue Heron

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes			Oligo	Meso	Eutro	Dystro	
1	Trophic Status is determined DOC in Epiliminon as:		<3	3-5	5-10	10+	mg DOC/L
	from Wetzel	Flag	1	2	3	4	
2	Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)
HgII	mean	3.8	5.3	4.9	5.4
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6
	n	17	35	2	3
MeHg	mean	2.8	4.9	3.9	5
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5
	n	11	2		

Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
6309.573	199526.23	79432.82	251188.64	1.5	299289.3	349170.9	
630957.3	7943282.3	1000000	398107.17	2	399052.5		15,886,565
			199526.23				
630.9573	79432.823	7943.282	100000	5	397164.1	516313.4	
	1584893.2	100000	316227.77	8	635462.6		12,679,146
			630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.74E-07	0.47
C_HgII_1_Aq			g/m3	9.64E-08	0.10
C_MeHg_1_Aq			g/m3	3.79E-08	0.04
C_Hg0_2_Aq			g/m3	1.43E-06	1.43
C_HgII_2_Aq			g/m3	3.08E-06	3.08
C_MeHg_2_Aq			g/m3	2.86E-07	0.29
C_Hg0_pore			g/m3	1.43E-06	1.43
C_HgII_pore			g/m3	3.60E-06	3.60
C_MeHg_pore			g/m3	6.35E-08	0.06
C_HgT_1_filtered			g/m3	6.08E-07	0.61
C_HgT_2_filtered			g/m3	4.79E-06	4.79
C_HgT_Sed_filtered			g/m3	5.10E-06	5.10
C_Hg0_1_T			g/m3	4.74E-07	0.47
C_HgII_1_T			g/m3	1.87E-06	1.87
C_MeHg_1_T			g/m3	2.07E-07	0.21
C_Hg0_2_T			g/m3	1.43E-06	1.43
C_HgII_2_T			g/m3	7.69E-06	7.69
C_MeHg_2_T			g/m3	3.40E-07	0.34
C_Hg0_sed, bulk			g/m3	1.19E-06	1
C_HgII_1_sed, bulk			g/m3	2.27E-01	226,907
C_MeHg_1_sed, bulk			g/m3	4.65E-04	465
C_Hg0_sed, wet			g/g	9.27E-13	0.000
C_HgII_1_sed, wet			g/g	2.72E-07	0.272
C_MeHg_1_sed, wet			g/g	4.22E-14	0.000
C_HgT_sed,wet			g/g	2.72E-07	0.272
C_Hg0_sed, dry weight			g/g	2.63E-12	0.0000
C_HgII_1_sed, dry weight			g/g	5.04E-07	0.5037
C_MeHg_1_sed, dry weight			g/g	1.03E-09	0.0010
C_HgT_1			g/m3	2.55E-06	2.551
C_HgT_2			g/m3	9.46E-06	9.457
C_HgT_Sed, dry weight			g/g	5.05E-07	0.505

		% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)	8.13%	73.29%	18.58%
Layer 2		3.60%	81.28%	15.12%
Sediments		0.20%	99.80%	0.00%

Q'	Bulk Exchange Flow	m3/yr	3,017,619
Qin	Inflow	m3/yr	3,474,314
Qout	Outflow	m3/yr	3,474,314
Aw	Surface Area of the Water Body	m2	378,381
E	Exchange rate	m2/yr	2
V_1	Volume of Layer 1	m3	183,741
V_2	Volume of Layer 2	m3	37,838
z1	depth of first water layer	m	0.49
z2	depth of second water layer	m	0.10

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.009
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.031
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.069
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.141
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.043
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.152
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.331
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.700

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi}V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{s1} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{s1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	4.740E-07
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.870E-06
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	2.074E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.430E-06
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	7.687E-06
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T	3.402E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	1.187E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.27E+08	0.00E+00	0.00E+00	-4.29E+03	2.89E+00	0.00E+00	C_HgII_1_sed	2.269E-01
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	4.648E-04

Inverted Matrix

-1.21E-08	-1.12E-08	-5.13E-09	-1.14E-08	-1.13E-08	-5.60E-09	-1.14E-08	-1.13E-08	-5.60E-09	4.74001E-07
-2.70E-08	-4.47E-08	-1.21E-08	-3.98E-08	-4.17E-08	-1.42E-08	-3.98E-08	-4.17E-08	-1.42E-08	1.86967E-06
-7.21E-10	-1.15E-09	-1.60E-07	-2.55E-09	-2.83E-09	-1.48E-07	-2.55E-09	-2.88E-09	-1.48E-07	2.07388E-07
-2.197E-08	-3.407E-08	-1.369E-08	-1.17E-07	-8.15E-08	-2.15E-08	-1.17E-07	-8.14E-08	-2.15E-08	1.4299E-06
-1.147E-07	-1.835E-07	-6.226E-08	-4.06E-07	-4.50E-07	-8.83E-08	-4.06E-07	-4.50E-07	-8.85E-08	7.68731E-06
-2.334E-09	-3.731E-09	-1.856E-07	-8.26E-09	-9.16E-09	-4.79E-07	-8.26E-09	-9.32E-09	-4.78E-07	3.40213E-07
-1.82E-08	-2.83E-08	-1.14E-08	-9.73E-08	-6.76E-08	-1.78E-08	-4.02E-06	-6.76E-08	-1.79E-08	1.18682E-06
-3.39E-03	-5.42E-03	-1.84E-03	-1.20E-02	-1.33E-02	-2.61E-03	-1.20E-02	-1.35E-02	-2.61E-03	0.226906529
-3.80E-06	-6.08E-06	-2.13E-04	-1.35E-05	-1.49E-05	-5.48E-04	-1.35E-05	-1.52E-05	-7.79E-04	0.000464799

x=b/A

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.005
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.062
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.099
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.794
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.049
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.025
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.538
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.159
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		1.32E-05
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		1.13E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}} \cdot \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.58
C_HgII_1_Aq			g/m3	2.97E-06	2.97
C_MeHg_1_Aq			g/m3	7.43E-07	0.74
C_Hg0_2_Aq			g/m3	1.10E-04	110.39
C_HgII_2_Aq			g/m3	2.44E-04	244.01
C_MeHg_2_Aq			g/m3	1.08E-05	10.76
C_Hg0_pore			g/m3	1.10E-04	110.39
C_HgII_pore			g/m3	2.91E-04	290.76
C_MeHg_pore			g/m3	2.84E-06	2.84
C_HgT_1_filtered			g/m3	1.93E-05	19.29
C_HgT_2_filtered			g/m3	3.65E-04	365.17
C_HgT_Sed_filtered			g/m3	4.04E-04	403.99
C_Hg0_1_T			g/m3	1.56E-05	15.58
C_HgII_1_T			g/m3	5.77E-05	57.66
C_MeHg_1_T			g/m3	4.06E-06	4.06
C_Hg0_2_T			g/m3	1.10E-04	110.39
C_HgII_2_T			g/m3	6.10E-04	609.90
C_MeHg_2_T			g/m3	1.28E-05	12.80
C_Hg0_sed			g/m3	9.16E-05	91.63
C_HgII_1_sed			g/m3	1.83E+01	18314487.35
C_MeHg_1_sed			g/m3	2.08E-02	20771.02
C_Hg0_sed, wet			g/g	3.46E-11	0.000
C_HgII_1_sed, wet			g/g	1.43E-05	14.303
C_MeHg_1_sed, wet			g/g	2.49E-08	0.025
C_HgT_sed,wet			g/g	1.43E-05	14.328
C_Hg0_sed, dry weight			g/g	2.03E-10	0.00
C_HgII_1_sed, dry weight			g/g	4.07E-05	40.65
C_MeHg_1_sed, dry weight			g/g	4.61E-08	0.05
C_HgT_1			g/m3	7.73E-05	77.30
C_HgT_2			g/m3	7.33E-04	733.10
C_HgT_Sed			g/g	4.07E-05	40.70
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		5.25%	74.59%	20.15%
Layer 2			1.75%	83.19%	15.06%
Sediments			0.11%	99.89%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.88548%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	3.06930%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	6.87088%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	4.27053%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	15.22372%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	33.13706%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.02796%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{Hg1,1} + \left[kw_{mer} \cdot V_w + kw_{photorad} \cdot V_w\right] \cdot C^w_{MeHg,1} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg,1} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{metR} \cdot V_w - v_{s,1} \cdot f^{w,1}_{abioHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg,1}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{metR} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} V_w - v_{s,1} \cdot f^{w,1}_{abioMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg,1} + Q' \cdot C^w_{MeHg,2}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg,2} + \left[-Q' - kw_{oxid} V_w - v_{s,1} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg,2} + \left[-Q' - kw_{red,2} \cdot V_w - kw_{metR} \cdot V_w - v_{s,1} \cdot f^{w,2}_{abioHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg,2}}{dt} = +\left[kw_{red,2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photorad} \cdot V_w - v_{s,1} \cdot f^{w,2}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioMeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg,2} + Q' \cdot C^w_{MeHg,3} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,1} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,1} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,1} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - \left(v_{rs} + v_b\right) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E-01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.57E-01	C_MeHg_1_T
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix										x=b/A
1.558E-05	-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.34E-07	-2.77E-09	1.56E-05	
5.766E-05	-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.78E-09	5.77E-05	
4.061E-06	-9.27E-17	-3.53E-16	-1.59E-07	7.27E-15	-4.95E-16	-1.47E-07	8.42E-13	2.13E-07	-1.47E-07	4.06E-06	
1.104E-04	-1.569E-09	-1.446E-09	-1.353E-09	4.51E-08	-1.40E-09	-2.51E-09	-4.51E-08	6.02E-06	-1.11E-09	0.00011	
6.099E-04	-1.979E-09	-3.165E-09	5.934E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.33E-05	2.43E-08	0.00061	
1.280E-05	7.949E-17	-4.998E-16	-1.842E-07	2.36E-14	-1.59E-15	-4.76E-07	2.72E-12	6.88E-07	-4.76E-07	1.28E-05	
9.163E-05	-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.20E-10	9.16E-05	
1.831E+01	1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.44E-04	3.95E-06	9.99E-01	7.75E-04	18.31449	
2.077E-02	5.27E-13	-1.69E-13	-2.10E-04	3.95E-11	-1.42E-12	-5.44E-04	4.44E-09	1.12E-03	-7.75E-04	0.020771	

A*x=b

C_T_sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.98867%
L_T,Hg0	Total Load, Hg0		g/yr	3.99E-01
L_T,HgII	Total Load, HgII		g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg		g/yr	7.43E-01
Rate Constants				
kw_v,Hg0	water column volatilization loss rate constant, Hg0		per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII		per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg		per yr	0.65
kw_oxid_1	water column oxidation rate constant		per yr	610.22
kw_oxid_2	water column oxidation rate constant		per yr	525.60
kw_red_1	water column reduction rate constant, layer 2		per yr	246.95
kw_red_2	water column reduction rate constant, layer 2		per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1		per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2		per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1		per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2		per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1		per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2		per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant		per yr	0.00
kb_oxid	benthic oxidation rate constant		per yr	0.00
kb_red	benthic reduction rate constant		per yr	0.00
kb_methy	benthic methylation rate constant		per yr	0.00
kb_demeth	benthic demethylation rate constant		per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant		per yr	0.00
v_sA	abiotic settling velocity		m/yr	4792.628412
v_sB	biotic settling velocity		m/yr	73
v_rs	resuspension velocity		m/yr	0.003700005
k_mort	phytoplankton mortality rate		per yr	10.95
v_min	mineralization rate		per yr	0.01
v_bur	burial rate		m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	7.90
TSS+2			mg/L	0.56
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_Hg0_1	Effective K for Hg0 in layer 2		L/kg	2.33E+06
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.66E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	3.37E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \times 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio}^{j} C_{abio,i}^{j} + S_{org}^{j} C_{org,i}^{j} + S_{phyto}^{j} C_{phyto,i}^{j} + S_{zoo}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{\frac{TSS}{C_{filtered,i}^{j}}}$$

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Little Blue Heron

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	3.75E-06	3.75
C_HgII_1_Aq			g/m3	7.20E-07	0.72
C_MeHg_1_Aq			g/m3	1.91E-07	0.19
C_Hg0_2_Aq			g/m3	2.51E-05	25.06
C_HgII_2_Aq			g/m3	5.53E-05	55.33
C_MeHg_2_Aq			g/m3	2.56E-06	2.56
C_Hg0_pore			g/m3	2.51E-05	25.06
C_HgII_pore			g/m3	6.59E-05	65.88
C_MeHg_pore			g/m3	6.65E-07	0.66
C_HgT_1_filtered			g/m3	4.66E-06	4.66
C_HgT_2_filtered			g/m3	8.29E-05	82.95
C_HgT_Sed_filtered			g/m3	9.16E-05	91.61
C_Hg0_1_T			g/m3	3.75E-06	3.75
C_HgII_1_T			g/m3	1.40E-05	13.97
C_MeHg_1_T			g/m3	1.04E-06	1.04
C_Hg0_2_T			g/m3	2.51E-05	25.06
C_HgII_2_T			g/m3	1.38E-04	138.29
C_MeHg_2_T			g/m3	3.04E-06	3.04
C_Hg0_sed			g/m3	2.08E-05	20.80
C_HgII_1_sed			g/m3	4.15E+00	4,149,629.37
C_MeHg_1_sed			g/m3	4.87E-03	4,868.69
C_Hg0_sed, wet			g/g	7.85E-12	0.00
C_HgII_1_sed, wet			g/g	3.24E-06	3.24
C_MeHg_1_sed, wet			g/g	5.83E-09	0.01
C_HgT_sed,wet			g/g	3.25E-06	3.25
C_Hg0_sed, dry weight			g/g	4.62E-11	0.00
C_HgII_1_sed, dry weight			g/g	9.21E-06	9.21
C_MeHg_1_sed, dry weight			g/g	1.08E-08	0.01
C_HgT_1			g/m3	1.88E-05	18.76
C_HgT_2			g/m3	1.66E-04	166.40
C_HgT_Sed, dry weight			g/g	9.22E-06	9.22
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		5.56%	74.45%	19.99%
Layer 2			1.83%	83.11%	15.06%
Sediments			0.12%	99.88%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
z2	depth of second water layer		m	0	
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%	
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%	
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%	
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%	
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%	
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1			4.27053%	
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%	
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%	
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2			33.13706%	
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%	

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{2A} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{2B} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII,1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{meth} \cdot V_w - v_{2A} \cdot f^{w,1}_{abiaHgII} A_w - v_{2B} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII,1} + Q' \cdot C^w_{HgII,2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII,1} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{2A} \cdot f^{w,1}_{abiaMeHg} \cdot A_w - v_{2B} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[kw_{mer} \cdot V_w + kw_{photored2} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{2A} \cdot f^{w,2}_{abiaHg0} \cdot A_w - v_{2B} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{2w} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{2w} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{r2} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII,2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{2A} \cdot f^{w,2}_{abiaHgII} A_w - v_{2B} \cdot f^{w,2}_{bioHgII} A_w - R_{2w} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII,2} + Q' \cdot C^w_{HgII,1} + \left[R_{2w} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{r2} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{meth2} \cdot V_w\right] \cdot C^w_{HgII,2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} \cdot V_w - v_{2A} \cdot f^{w,2}_{abiaMeHg} \cdot A_w - v_{2B} \cdot f^{w,2}_{bioMeHg} A_w - R_{2w} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{2w} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{r2} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{2w} f^{w,2}_{aqHg0} + \left(v_{2A} \cdot f^{w,2}_{abiaHg0} + v_{2B} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{2w} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{r2} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{2w} f^{w,2}_{aqHgII} + \left(v_{2A} \cdot f^{w,2}_{abiaHgII} + v_{2B} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} \cdot V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{2w} \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{r2} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{2w} f^{w,2}_{aqMeHg} + \left(v_{2A} \cdot f^{w,2}_{abiaMeHg} + v_{2B} \cdot f^{w,2}_{bioMeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{2w} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{r2} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	3.750E-06
C_HgII_1_T	1.12E+08	-6.29E+07	4.02E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.397E-05
C_MeHg_1_T	0.00E+00	6.91E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	1.043E-06
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	2.506E-05
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	6.43E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	1.383E-04
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	6.43E-01	-8.19E+06	0.00E+00	4.31E+03	0.00E+00	0.00E+00	C_MeHg_2_T	3.043E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	2.080E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	4.15E+00	C_HgII_1_sed	4.150E+00
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	1.45E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	4.869E-03

Inverted Matrix										x=b/A
-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.34E-07	-2.77E-09	3.7E-06	
-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.78E-09	1.4E-05	
-9.27E-17	-3.53E-16	-1.59E-07	7.27E-15	-4.95E-16	-1.47E-07	8.42E-13	2.13E-07	-1.47E-07	1E-06	
-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.51E-09	-4.51E-08	6.02E-06	-1.11E-09	2.5E-05	
-1.979E-09	-3.165E-09	5.934E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.33E-05	2.43E-08	0.00014	
7.949E-17	-4.998E-16	-1.842E-07	2.36E-14	-1.59E-15	-4.76E-07	2.72E-12	6.88E-07	-4.76E-07	3E-06	
-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.20E-10	2.1E-05	
1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.44E-04	3.95E-06	9.99E-01	7.75E-04	4.14963	
5.27E-13	-1.69E-13	-2.10E-04	3.95E-11	-1.42E-12	-5.44E-04	4.44E-09	1.12E-03	-7.75E-04	0.00487	

A*x=b

Target C_sed, wet 4.154518855 g/g

APPENDIX C
MODEL INPUTS AND OUTPUTS
SCENARIO 2
Little Blue Heron

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate c	per yr	388.36
kw_v,HgII	water column volatilization loss rate c	per yr	0.00
kw_v,MeHg	water column volatilization loss rate c	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant	per yr	246.95
kw_red_2	water column reduction rate constant	per yr	107.40
kw_meth_1	water column methylation rate consta	per yr	0.00
kw_meth_2	water column methylation rate consta	per yr	0.00
kw_demeth_1	water column demethylation rate con	per yr	0.00
kw_demeth_2	water column demethylation rate con	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for	per yr	6.43
kw_mer	water column *mer* cleavage demeth	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeH	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed} \cdot 3.1536\text{x}10^7}{z_{sed}}$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j} + S_{org}^{j}C_{org,i}^{j} + S_{phyto}^{j}C_{phyto,i}^{j} + S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}} \Big/ \frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS} = \frac{TSS}{C_{filtered,i}^{j}}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w} \right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2} \right) Sc_{w,i}^{-0.67} \left(3.15 x 10^{7} \right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2} \right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{\nu_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$\nu_a = \left(1.32 + 0.009 \bullet T_a\right) x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27053%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			33.13706%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.53471%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			6.15876%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00410%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.92923%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			79.43383%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			4.94622%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			53.83330%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			2.46695%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.98867%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.31
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.44
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	2,743.46
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}+K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}+K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}+K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo}+K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto}+K_{bio\_dead,i}^{aq}\cdot S_{bio,dead}+K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed}+K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6}+K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	7.90	mg/L
Sbio_zoo,1	2.5		TSS_2	0.56	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	3.11E-01				
Sbio_dead,2	4.37E-01				
S_abio, sed	5.28E+04				
S_bio_dead,sed	2.74E+03				
S_sed,total	5.56E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

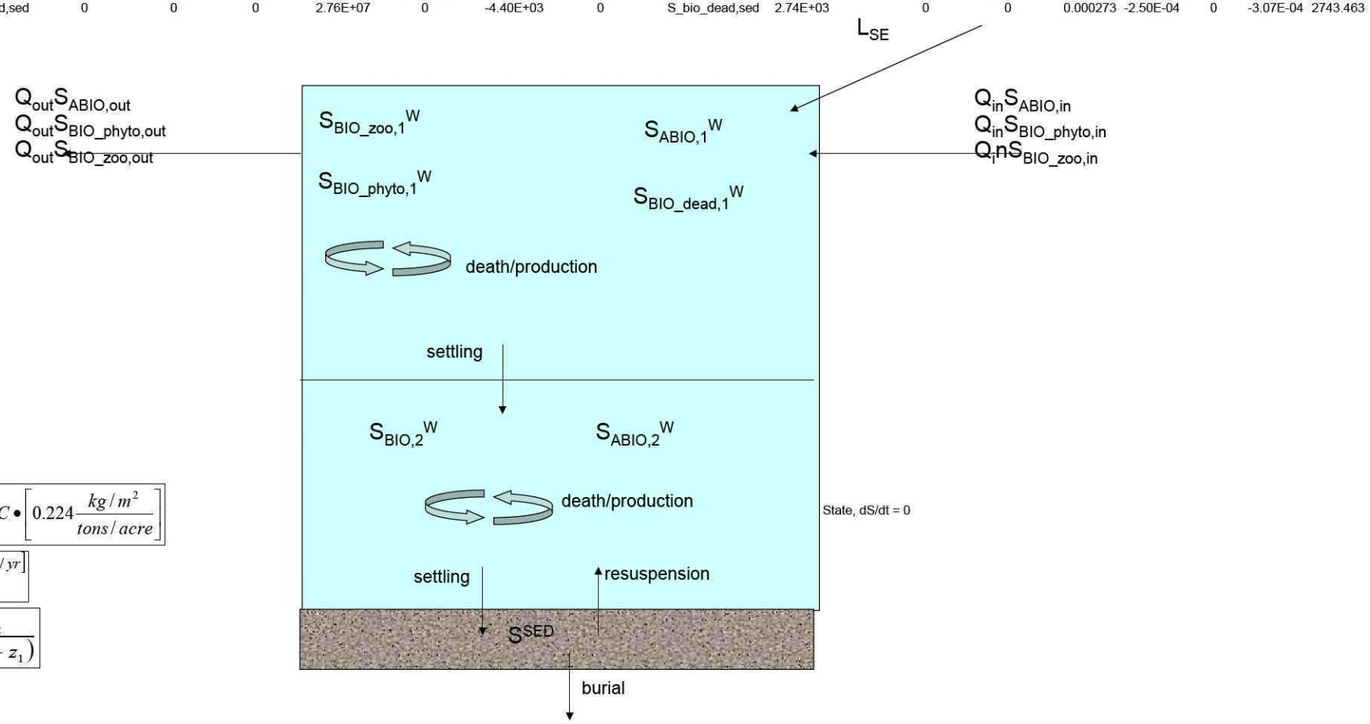
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	1.01E+07	S_bio_dead,1	3.11E-01	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.311342
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	4.37E-01	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.4367
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	2.74E+03	0	0	0.000273	-2.50E-04	0	-3.07E-04	2743.463



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	1.16364E-07	1	2
k_meth_2	abiotic* methylation in layer 2		per day	1.16364E-06	1	4
k_meth_1	abiotic methylation in layer 1		per yr	4.24727E-05		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000424727		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00885	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.06871		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.04271		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.33137		
k_meth_1	abiotic methylation in layer 1		per yr	3.76E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	1.70E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	3.49091E-07	1	2
k_meth_b	biotic methylation in sediments		per yr	0.000127418		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	1.16364E-08	1
k_demeth_2	biotic demethylation in layer 2		per day	1.16364E-07	
k_demeth_1	biotic demethylation in layer 1		per yr	4.24727E-06	
k_demeth_2	biotic demethylation in layer 2		per yr	4.24727E-05	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.85E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			3.31E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	2.19E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	1.70E-05	

$$k_{demeth} = k_{demeth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC} \right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608.
mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	6.98182E-07	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.000254836		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{1.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43* ,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids. This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1. Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM. In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem, which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1. For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60) For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific Application of SERAFM	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b. Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening). BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet. In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations. The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1). The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Scenario 2 – Mink

Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury Beta Version: 1.0.4a Last Revision 08/08/2007

Watershed Characteristics

	Value	Units	Notes
Watershed Location (East or West)	East		0
Watershed Area (as Contributing Area)	647,500	m2	
Percent Impervious	2.1%	--	
Percent Wetland	53.3%	--	
Percent Riparian	13.3%	--	
% with Known Contaminated Soil	15.6%	--	
Percent Upland	15.7%	--	1
Lake Area	378,381	m2	
Epilimnion Depth	0.49	m	
Hypolimnion Depth	0.1	m	2
Anoxic Hypolimnion	YES	--	3
Hydraulic Residence Time		yr	4
Inflow	3.47E+06		
Outflow	3.47E+06	m3/yr	
Water pH	7.15	--	
Epilimnion Water Temp	29.39	C	
Hypolimnion Water Temp	29.39	C	
Air Temp	19.9	C	
Annual Precipitation	105.2	cm/yr	
DOC Epilimnion	16	mg/L	
DOC Hypolimnion	16	mg/L	
Color (as PtCo)	0	PtCo	
Trophic Status	Eutrophic		

Inflow Mercury Concentrations

Hg0	0	g/m3		
HgII	5.64E-06	g/m3	5.64	35.58437977
MeHg	7.33E-08	g/m3	0.07332	83.29934922

Total Mercury Concentration in Contaminated Sediment, dry weight	40.7 ug/g

Known Mercury in Contaminated Soils

Cs,Hg0	0	g/m3
Cs,HgII	1.129080624	g/m3
Cs,MeHg	4.13E-03	g/m3

Required Hazard Index for Sensitive Indicator	1

Kd_abio			
HgII	7,182,936	1	
MeHg	15,887	1	
Kd_bio			
HgII	17,941,378	1	
MeHg	2,581,565	1	
Kd_DOC			
HgII	301,427	1	
MeHg	310,000	1	
	PCT ERROR	CLEANUP	
MeHg Filtered	-23.71	16.54	
HgT Filtered	-22.10		
MeHg Unfilter	-49.61		
HgT Unfiltere	237.77		

Exposure Concentrations

		Scenario 1: With Contaminated Sediment	Units	Measured Concentrations	Absolute Error	Relative Error	Scenario 2: Background Conditions		Scenario 3: Conditions at Proposed Target-Levels	
Epilimnion	Hg0 Filtered	15.61	ng/L		-15.61	-100	0.47	ng/L	6.51	ng/L
	HgII Filtered	2.97	ng/L		-2.97	-100	0.10	ng/L	1.24	ng/L
	MeHg Filtered	1.01	ng/L	0.77	-0.24	-23.71046	0.04	ng/L	0.43	ng/L
	HgT Filtered	19.59	ng/L	15.26	-4.33	-22.10485	0.61	ng/L	8.18	ng/L
	Hg0 Unfiltered	15.61	ng/L		-15.61	-100	0.47	ng/L	6.51	ng/L
	HgII Unfiltered	57.70	ng/L		-57.70	-100	1.87	ng/L	24.14	ng/L
	MeHg Unfiltered	5.52	ng/L	2.78	-2.74	-49.61463	0.23	ng/L	2.34	ng/L
	HgT Unfiltered	78.82	ng/L	266.23	187.41	237.76746	2.56	ng/L	32.99	ng/L
Hypolimnion	Hg0 Filtered	110.40	ng/L		-110.40	-100	1.42	ng/L	44.90	ng/L
	HgII Filtered	243.91	ng/L		-243.91	-100	3.06	ng/L	99.14	ng/L
	MeHg Filtered	14.72	ng/L		-14.72	-100	0.33	ng/L	6.08	ng/L
	HgT Filtered	369.04	ng/L		-369.04	-100	4.81	ng/L	150.12	ng/L
	Hg0 Unfiltered	110.40	ng/L		-110.40	-100	1.42	ng/L	44.90	ng/L
	HgII Unfiltered	609.66	ng/L		-609.66	-100	7.64	ng/L	247.81	ng/L
	MeHg Unfiltered	17.52	ng/L		-17.52	-100	0.40	ng/L	7.23	ng/L
	HgT Unfiltered	737.58	ng/L		-737.58	-100	9.46	ng/L	299.94	ng/L
	Sediment									
	Hg0 porewater	110.40	ng/L		-110.40	-100	1.42	ng/L	44.900	ng/L
	HgII porewater	290.64	ng/L		-290.64	-100	3.58	ng/L	118.099	ng/L
	MeHg porewater	3.88	ng/L		-3.88	-100	0.08	ng/L	1.595	ng/L
	HgT porewater	404.93	ng/L		-404.93	-100	5.08	ng/L	164.594	ng/L
	Hg0 bulk, dry	0.00	ug/g		0.00	-100	0.00	ug/g	0.00	ug/g
	HgII bulk, dry	40.64	ug/g		-40.64	-100	0.27	ug/g	16.51	ug/g
	MeHg bulk, dry	0.06314	ug/g	0.00658	-0.06	-89.57908	0.00	ug/g	0.03	ug/g
	HgT bulk, dry	40.70	ug/g	40.7	0.00	0	0.502	ug/g	16.54	ug/g
Fish	Trophic Level 3	0.92	ug/g		-0.92	-100	0.038	ug/g	0.39	ug/g
	Trophic Level 4	2.01	ug/g		-2.01	-100	0.082	ug/g	0.85	ug/g
	HI	2.36					0.10		1.00	
	Sensitive Indicator	Mink					Mink		Mink	
	Target C_sed, dry	16.54	ug/g	Note: 8						
	Target C_sed, wet	7.45	ug/g							

Rate Constants

Process	Media	Value	Units	
Methylation	Epilimnion	1.60E-07	per day	1.60E-04
	Hypolimnion	1.60E-06	per day	
	Sediment	4.80E-07	per day	
Demethylation	Epilimnion	1.60E-08	per day	
	Hypolimnion	1.60E-07	per day	
	Sediment	9.60E-07	per day	
Biotic Reduction	Water Column	0.03	per day	
Photo-Degradation (MeHg --> Hg0)	Water Column	0.002	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) Visible Light	Water Column	0.03	per day per E/m2-day	
Photo-Reduction (HgII --> Hg0) UV-B	Water Column	28.25	per day per E/m2-day	
Photo-Oxidation (Hg0 --> HgII) UV-B	Water Column	58.85	per day per E/m2-day	
Dark Oxidation	Water Column	1.44	per day	

Trophic Level 1 BAF: Phytoplankton	Phyto	1.89E+05
Trophic Level 2 BAF: Aq insects	Aq Insects	1.67E+05
Trophic Level 2 BAF: Crayfish and Frog	Crayfish and Frog	1.80E+05
Trophic Level 3 BAF: Fish	Fish	9.14E+05
Trophic Level 4 BAF : Fish	Fish	1.99E+06

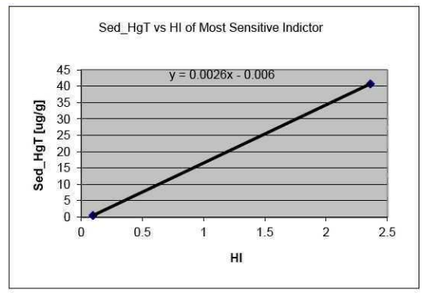
Human and Wildlife Exposure Risk Results

6,250

	Hazard Quotient		
	Contaminated	Background	for Proposed Target-Level
Wildlife			
Little Brown Bat	1.13	0.05	0.48
Otter	1.22	0.05	0.51
Mink	**2.36**	0.10	1.00
Great Blue Heron	0.00	0.00	0.00
Little Blue Heron	0.00	0.00	0.00
Pied-bill Grebe	**2.16**	0.09	0.92
Kingfisher	0.00	0.00	0.00
Wood Duck	0.84	0.03	0.36
Alligator	0.00	0.00	0.00
Human			
Man	0.00	0.00	0.00
Woman	0.00	0.00	0.00
Adult	0.00	0.00	0.00
Child	0.00	0.00	0.00
Native American	0.00	0.00	0.00

Indicates an exceedence of HI=1

x	y
HI	Sed_HgT
2.36	40.70
0.10	0.50
m =	17.746
b=	-1.207
Sed_HgT	16.538
for HI =	1



Notes

1 Calculated for user as the remainder of watershed area.
2 If you are modeling a river or a well-mixed lake, enter 0.1
3 Type 'YES or 'NO to flag whether the hypolimnion is anoxic or not. If it is anoxic, then methylation will default to a faster rate in the hypolimnion (k_meth = 0.01/d anoxic, 0.001/d oxic).
4 Used to calculate inflow and outflow, if there are seepage or ground water inputs, then Qin and Qout can be hard coded
5 Color is required in terms of PtCo. If PtCo>50 then the lake is classified as dystrophic, if user does not know, then enter 0
6 If this is not the trophic status you believe your waters to be, then this can be hardcoded/overwritten by going to the Parameters sheet and updating the number for trophic status flag.
7 If the user has contaminated soil concentrations in the watershed, then the percent of the watershed can be used to override the calculations of watershed export. The soil concentration is then used for soil erosion and runoff.
8 The Target sediment concentration is estimated using a linear relationship between the background conditions and the contaminated conditions. This will most likely cause HI to be near, but not quite equal to, unity.
An exact result can be found by using the "Goal Seek" function under tools.
Use "Set Cell" to Q38, "to value" to B43, and "By Changing Cell" to H41

$$\text{Absolute Error} = \text{Observed} - \text{Predicted}$$

$$\text{Relative Error} = \frac{\text{Observed} - \text{Predicted}}{\text{Observed}} \bullet 100\%$$

	Site-Specific User Input	Required
	Model Calculated	No input required
	Data Necessary for certain sites	Only necessary if applicable to site of interest
	Scenario 1 Output	
	Scenario 2 Output	
	Scenario 3 Output	

Predicted Mercury Concentrations in Fish and Wildlife and Hazard Quotients

Scenario	Contaminated Sediment	Uncontaminated Sediment	Target	
Water Concentration [MeHg]	1.01	0.04	0.427	ng/L

Biota

Trophic Level 1: Phytoplankton	0.19	0.01	0.08	ug Hg/ g wet weight
Trophic Level 2: Insects	0.17	0.01	0.07	ug Hg/ g wet weight
Trophic Level 2: Crayfish	0.18	0.01	0.08	ug Hg/ g wet weight
Trophic Level 3 : Bluegill	0.92	0.04	0.39	ug Hg/ g wet weight
Trophic Level 4: Bass	2.01	0.08	0.85	ug Hg/ g wet weight
Trophic Level 3: Silverside	1.09	0.04	0.46	ug Hg/ g wet weight
Trophic Level: 3 Crayfish	0.19	0.01	0.08	ug Hg/ g wet weight
Trophic Level 3: Bullfrog	0.18	0.01	0.07	ug Hg/ g wet weight

Note: These numbers call the BAFs from the Input&Output spreadsheet

$$Potential\ Dose = \frac{Conc \bullet IngestionRate}{BodyWeight}$$

$$Total\ Dose = \sum \%Diet_{trophiclevel_i} \bullet Potential\ Dose_i + \left(drinking\ rate \bullet [Hg]_{water}\right)$$

$$HQ = \frac{Total\ Dose}{TRV\ or\ RfD}$$

These tables present the potential dose calculations for each trophic level, the total dose, and the hazard quotients for the three given scenarios: contaminated sediment, natural (background) conditions, and the proposed clean-up level condition.

Wildlife	Body Weight	Ingestion Rate	Drinking rate	Percent of Diet from Trophic Level 1 : Phytoplankton and Plants	Percent of Diet from Trophic Level 2 : Insects	Percent of Diet from Trophic Level 2 : Crayfish or Frogs	Percent of Diet from Trophic Level 3 : Fish	Percent of Diet from Trophic Level 4 : Fish	Percent of Diet from nonaquatic sources	Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Insects	Potential Dose from Trophic Level 2: Crayfish	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
Animal	[kg in wet weight]	[kg wet weight/d]	[L/d]	--	--	--	--	--	--	[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
Little Brown Bat	0.0075	0.00377	0.0012	0%	100%	0%	0%	0%	0%	0	0	85	0	0	0	85	75	**1.13**
Otter	7.4	0.733	0.62	0%	0%	15%	75%	10%	0%	0	0	0	3	69	20	91	75	**1.22**
Mink	0.85	0.1145	0.085	0%	0%	35%	5%	60%	0%	0	0	0	9	6	162	177	75	**2.36**
Great Blue Heron	2.2	0.509	0.1	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Little Blue Heron	0.34	0.147	0.16	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Pied-bill Grebe	0.417	0.168	0.03	0%	60%	20%	20%	0%	0%	0	0	41	15	74	0	130	60	**2.16**
Kingfisher	0.15	0.086	0.017	0%	0%	0%	0%	0%	100%	0	0	0	0	0	0	0	60	0.00
Wood Duck	0.673	0.1834	0.045	75%	25%	0%	0%	0%	0%	0	39	11	0	0	0	50	60	0.84
Alligator	50	0.80	0.000	0%	0%	35%	17%	48%	0%	0	0	0	1	3	15	19	5000	0.00
Human																	RfD	
Man	78	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Woman	65	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Adult	70	0.0066	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
Child	45	0.0066	0.9	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
Native American	70	0.059	1.4	0%	0%	0%	0%	0%	100%	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

from: Mercury Report to Congress, Volume VI, Section 3.3. Table
and cited in: Nichols,J.,S. Bradbury, J. Swartout. 1999. Derivation of Wildlife Values for Mercury. Journal of Toxicology and Environmental Health, Part B. 2:325-255.
TRV values from Nichols, et al. 1999. Avian species: 13 ug/kg/d; mammalian species: 16 ug/kg/d.
Human values are from Exposure Factors Handbook. Child drinking rate is the average of children 1-10 (.74 L/d) and 11-19 (0.97 L/d).
Percent Diet of Trophic Level 4 fish is assumed because the ingestion rate is fish specific. It is assumed that all the fish ingested of this type are exposed to the contamination and are of trophic level 4.
Woman modeled as pregnant or child-bearing age
TRV Toxicity Reference Value

Methylmercury Bioaccumulation Factors

	Percentile of Distribution				
	5th	25th	50th	75th	95th
Trophic Level 1: Phyto			1.89E+05		
Trophic Level 2: Insects			1.67E+05		
Trophic Level 2: Crayfish and Frog			1.80E+05		
Trophic Level 3: Bluegill			9.14E+05		
Trophic 4: Bass	3.30E+06	5.00E+06	1.99E+06	9.20E+06	1.40E+07
Trophic 3: Brook Silver Side			1.08E+06		
Trophic: 3 Crayfish			1.87E+05		
Trophic 3: Bullfrog			1.74E+05		

$$BAF = \frac{\frac{ug}{kg}}{\frac{ug}{L}}$$

Background conditions: Condition of Site under only atmospheric loading

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.007	0.00	3.46	0.00	0.00	0.00	3	75	0.05
0.003	0.00	0.00	0.11	2.80	0.81	4	75	0.05
0.004	0.00	0.00	0.35	0.25	6.62	7	75	0.10
0.002	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.019	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.003	0.00	1.66	0.60	3.03	0.00	5	60	0.09
0.005	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.003	1.59	0.47	0.00	0.00	0.00	2	60	0.03
0.000	0.00	0.00	0.04	0.10	0.63	1	5000	0.00
							RfD	
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.001	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Concentrations at Proposed Target-Level Conditions

Potential Dose from Water	Potential Dose from Trophic Level 1	Potential Dose from Trophic Level 2: Zooplankton	Potential Dose from Trophic Level 2: Benthos	Potential Dose from Trophic Level 3	Potential Dose from Trophic Level 4	Total Potential Dose	TRV	HQ (Total Dose / TRV)
[ng/d/kg]	ug Hg / kg wet weight / d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	ug Hg/kg wet weight/d	--
0.068	0.00	35.88	0.00	0.00	0.00	36	75	0.48
0.036	0.00	0.00	1.14	29.02	8.42	39	75	0.51
0.043	0.00	0.00	3.63	2.63	68.74	75	75	1.00
0.019	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.201	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.031	0.00	17.25	6.20	31.48	0.00	55	60	0.92
0.048	0.00	0.00	0.00	0.00	0.00	0	60	0.00
0.029	16.51	4.86	0.00	0.00	0.00	21	60	0.36
0.000	0.00	0.00	0.43	1.06	6.52	8	5000	0.00
							RfD	
0.008	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.1	0.00
0.009	0.00	0.00	0.00	0.00	0.00	0.00	0.3	0.00

Water Body Hydrology

Symbol	Parameter	Equation	Units	Value	
Aw	Surface Area of the Water Body		m2	3.78E+05	Link
z_1	Thickness of Layer 1		m	4.86E-01	Link
z_2	Thickness of Layer 2		m	1.00E-01	Link
Vw_1	Volume of Layer 1	Aw*z_1	m3	1.84E+05	Calc
Vw_2	Volume of Layer 2	Aw*z_2	m3	3.78E+04	Calc
θ	Hydraulic Residence Time		yr	0	Link
Qin	Inflow		m3/yr	3.47E+06	Calc
Qout	Outflow		m3/yr	3.47E+06	Calc
Cin_Hg0	Inflow Hg0 Concentration		g/m3	0	User
Cin_HgII	Inflow HgII Concentration		g/m3	0.00000564	User
Cin_MeHg	Inflow MeHg Concentration		g/m3	7.332E-08	User
P	Average Annual precipitation		cm/yr	105.2	Link
E	*Average Annual evaporation*		*cm/yr*	*100*	*not currently used*
DOC_1	DOC in Layer 1		mg/L	16	Link
DOC_2	DOC in Layer 2		mg/L	16	Link
DOC_Sed	*DOC in Sediments*		*mg/L*	*10*	*not currently used*
TOC_Sed	*TOC in Sediments*		*g org C/m2*	*7.76*	*not currently used*
Trophic Level	Trophic Status, Flagged as 1-4			3	Comp
pH 1	pH in Layer 1			7.15	Link
pH 2	pH in Layer 2			7.15	Link
pH Sed	pH in sediments			7.15	Link

$$Q = \frac{V}{\theta}$$

Watershed Characteristics

Symbol	Parameter	Equation	Units	Value	
AC	Surface Area of the Catchment		m2	647,500	Link
Impr_%	Percent Impervious		--	2%	Link
Wetl_%	Percent Wetland		--	53%	Link
Ripar_%	Percent Riparian		--	13%	Link
Cont_%	Percent Known Contaminated Soils		--	16%	Link
Upland_%	Percent Upland (Remainder: 100% - others)		--	16%	Comp
Ac_imperv	Surface Area of Impervious Catchment		m2	13,598	Comp
Ac_wetland	Surface Area of Wetland		m2	345,118	Comp
Ac_ripar	Surface Area of Riparian		m2	86,118	Comp
Ac_cont_soil	Surface Area of Contaminated Soils		m2	101,010	Comp
Ac_updland	Surface Area of Upland		m2	101,658	Comp
zs	Depth of pervious soil layer		m	0.1	Default
ks_RO,Hg0	soil runoff rate constant, Hg0		per yr	0.001	Default
ks_RO,HgII	soil runoff rate constant, HgII		per yr	0.001	Default
ks_RO,MeHg	soil runoff rate constant, MeHg		per yr	0.001	Default
ks_e,Hg0	soil erosion loss rate constant, Hg0		per yr	0.0005	Default
ks_e,HgII	soil erosion loss rate constant, HgII		per yr	0	Default
ks_e,MeHg	soil erosion loss rate constant, MeHg		per yr	0	Default
Cs,Hg0	watershed soil concentration, Hg0		g/m3	0	Link: Input&Output
Cs,HgII	watershed soil concentration, HgII		g/m3	1.129080624	Link: Input&Output
Cs,MeHg	watershed soil concentration, MeHg		g/m3	0.004128952	Link: Input&Output
Part of Country	Eastern or Western		East		
Flag for Part of Cour	Eastern (1) or Western (2)		1		
u	avg wind speed 10 m above water surface		m/s	6	
R_Impervious, Hg0	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, HgII	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Impervious, MeH	Ratio of Export to Precipitation for Impervious Surface		--	1	
R_Wetland, Hg0	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, HgII	Ratio of Export to Precipitation for Wetlands		--	0.2	
R_Wetland, MeHg	Ratio of Export to Precipitation for Wetlands		--	4.9	
R_Riparian, Hg0	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, HgII	Ratio of Export to Precipitation for Riparian		--	0.2	
R_Riparian, MeHg	Ratio of Export to Precipitation for Riparian		--	2	
R_Upland, Hg0	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, HgII	Ratio of Export to Precipitation for Upland		--	0.2	
R_Upland, MeHg	Ratio of Export to Precipitation for Upland		--	0.2	

R values come from: Rudd, J.W.M. 1995. Sources of Methyl Mercury to Freshwater Ecosystems: A Review. Water, Air, and Soil Pollution. **80**: 697-713.

Water Body Characteristics

Symbol	Parameter	Equation	Units	Value		
T_1,C	Water body temperature, Layer 1, Celsius		Celsius	29.39	Link	
T_1,C	Water body temperature, Layer 2, Celsius		Celsius	29.39	Link	
T_1,K	Water body temperature, Layer 1, Kelvin		Kelvin	302.54	Comp	
T_2,K	Water body temperature, Layer 2, Kelvin		Kelvin	302.39	Comp	
T_a	air temperature, C		Celsius	19.9	Link	
Surface Light	Surface Light Intensity		E/m2-day	95.00	Default for 40deg Latitude	4
Cloud Cover	Fraction Cloud Reductance Factor		--	0.65		
Reflectance			--	0.05		
Percent Daylingt			--	0.50		
Surface Light	Surface Light Intensity: accounting for weather and refle		E/m2-day	29.33		5
ke	Light Extinction Coefficient		per m	2.25	Model	1,2
η UV-B layer 1	UV light extinction = f(DOC)		per m	76.66	Model	3
η UV-B layer 2	UV light extinction = f(DOC)		per m	76.66	Model	

Notes			Oligo	Meso	Eutro	Dystro	
1	Trophic Status is determined DOC in Epiliminon as:		<3	3-5	5-10	10+	mg DOC/L
	from Wetzel	Flag	1	2	3	4	
2	Light Extinction Coefficient		Oligo	Meso	Eutro	Dystro	
	from Wetzel		0.525	1.05	2.25	2.5	per m

3 from Scully and Lean: Scully, N.M., D.R.S. Lean, *Arch. Hydrobiol. Beih.* **1994**. 43,135. as cited by LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, and F.M.M.Morel. **2001**. Environ. Sci. Technol. *35*. 1367-1372.

4 from Zepp (1980), as cited in Mercury Report to Congress. Mean annual incident light at 40 deg latitude is 95 E/m2/day for clear skies

5 Assuming average cloud reduction facator of 0.65, a surface reflectance of 5%, and averaging half the day getting sunlight
Incident Light = Incident Light*reduction factor*(100%-surface reflectance)/100*(fraction daylight)

Basic Chemical Dependent Parameters: Hg0, HgII, MeHg

Units	MW g/mole	H atm-m3/mole	Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg	Kd_DOC L/kg	D_a,i cm2/sec	D_w,i cm2/sec
Hg0	201	7.10E-03	0	0	0	0	0	5.54E-02	6.41E-06
HgII	201	7.10E-10	6,310	7,182,936	260,558	17,941,378	301,427	5.54E-02	6.41E-06
MeHg	216	4.70E-07	631	15,887	4,557	2,581,565	310,000	5.28E-02	6.11E-06
MeHgCl	251							4.77E-02	5.53E-06
HgCl2	272	7.10E-10						4.53E-02	5.24E-06

Parameters

MW	molecular weight
H	Henry's Law Constant (NTG - appears to be from EPA Report to Congress)
Kd-soil	Soil-water partitiion coefficient
Kd-sed	Sediment-water partition coefficient
Kd_abio	Suspended sediment-water partition coefficient
Kd_bio	Suspended biotic solids-water partition coefficient
D_a,i	Diffusivity in air
D_w,i	Diffusivity in water

$$D_{a,i} = \frac{1.9}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

$$D_{w,i} = \frac{22x10^{-5}}{MW^{2/3}} \frac{cm^2}{\text{sec}}$$

Parameter values taken from the Mercury Report to Congress, 1997.

		Kd-soil L/kg	Kd_abio L/kg	Kd-sed L/kg	Kd_bio L/kg
HgII	Mean	58,000	50000	100,000	200,000
	Range	24,000 - 270,000	1,380 - 270,000	16,000 - 990,000	
MeHg	Mean	7000	3000	100,000	500,000
	Range	2,700 - 31,000	2,200 - 7,800	94,000 - 250,000	
Hg0		1,000	1,000	3000	1,000

Note: There is some research suggesting that the partition coefficients for mercury can be functions of pH (e.g., Hudson et al., 1994).
However the functionality is unclear, and the parameters must be site-specifically calibrated.
Therefore, we leave the direct calibration of the parameters to the user. This can be done by measuring mercury in filtered and unfiltered samples.

		Kd-soil log(L/kg)	Kd-suspended matter log(L/kg)	Kd-sediment log(L/kg)	DOC/Water log(L/kg)	Kd-soil L/kg	Kd-suspended matter L/kg	Kd-sediment L/kg	DOC/Water L/kg	multiplier for Kd_abio to Kd_bio	Kd-bio L/kg	Avg Kd_bio	NTG_max estimate of Kd_bio from Kd_suspended X max multiplier
HgII	mean	3.8	5.3	4.9	5.4	6309.573	199526.2	79432.82	251188.64	1.5	299289.3	349170.9	
	range	2.2-5.8	4.2-6.9	3.8-6.0	5.3-5.6	630957.3	7943282	1000000	398107.17	2	399052.5		15,886,565
	n	17	35	2	3				199526.23				
MeHg	mean	2.8	4.9	3.9	5	630.9573	79432.82	7943.282	100000	5	397164.1	516313.4	
	range	1.3-4.8	4.2-6.2	2.8-5.0	2.8-5.5		1584893	100000	316227.77	8	635462.6		12,679,146
	n	11	2						630.95734				

Allison, J.D. and T.L. Allison. 2000. Partition Coefficients for Metals in Surface Water, Soil, and Waste. Internal USEPA Report. 3169786.4

Mercury Report to Congress, 1997 cites R-MCM (Harris, et al., 1996) stating that
partitioning to biotics is 1.5 - 2times that of abiotics for HgII,and 5 - 8 times for MeHg

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	4.73E-07	0.47
C_HgII_1_Aq			g/m3	9.62E-08	0.10
C_MeHg_1_Aq			g/m3	4.12E-08	0.04
C_Hg0_2_Aq			g/m3	1.42E-06	1.42
C_HgII_2_Aq			g/m3	3.06E-06	3.06
C_MeHg_2_Aq			g/m3	3.34E-07	0.33
C_Hg0_pore			g/m3	1.42E-06	1.42
C_HgII_pore			g/m3	3.58E-06	3.58
C_MeHg_pore			g/m3	7.62E-08	0.08
C_HgT_1_filtered			g/m3	6.11E-07	0.61
C_HgT_2_filtered			g/m3	4.81E-06	4.81
C_HgT_Sed_filtered			g/m3	5.08E-06	5.08
C_Hg0_1_T			g/m3	4.73E-07	0.47
C_HgII_1_T			g/m3	1.87E-06	1.87
C_MeHg_1_T			g/m3	2.25E-07	0.23
C_Hg0_2_T			g/m3	1.42E-06	1.42
C_HgII_2_T			g/m3	7.64E-06	7.64
C_MeHg_2_T			g/m3	3.97E-07	0.40
C_Hg0_sed, bulk			g/m3	1.18E-06	1
C_HgII_1_sed, bulk			g/m3	2.26E-01	225,579
C_MeHg_1_sed, bulk			g/m3	5.58E-04	558
C_Hg0_sed, wet			g/g	9.22E-13	0.000
C_HgII_1_sed, wet			g/g	2.70E-07	0.270
C_MeHg_1_sed, wet			g/g	5.07E-14	0.000
C_HgT_sed,wet			g/g	2.70E-07	0.270
C_Hg0_sed, dry weight			g/g	2.62E-12	0.0000
C_HgII_1_sed, dry weight			g/g	5.01E-07	0.5007
C_MeHg_1_sed, dry weight			g/g	1.24E-09	0.0012
C_HgT_1			g/m3	2.56E-06	2.565
C_HgT_2			g/m3	9.46E-06	9.463
C_HgT_Sed, dry weight			g/g	5.02E-07	0.502
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		8.77%	72.77%	18.45%
Layer 2			4.20%	80.77%	15.03%
Sediments			0.25%	99.75%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	1.000
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.009
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	0.031
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	1.000
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	0.069
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	0.141
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.000
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1	0.043
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1	0.152
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.000
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2	0.331
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	0.700

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxi}V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} \cdot V_w - kw_{red,1} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioHgII} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHgII} \cdot A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{meth} \cdot V_w\right] \cdot C^w_{HgII} + \left[-Q_{out} - Q' - kw_{volMeHg} \cdot V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photorad} \cdot V_w - v_{s,A} \cdot f^{w,1}_{abioMeHg} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} \cdot A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} \cdot V_w + kw_{photorad} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s,A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{meth} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abiHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg2}}{dt} = +\left[kw_{meth,2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth2} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored2} \cdot V_w - v_{s,A} \cdot f^{w,2}_{abio,MeHg} \cdot A_w - v_{sB} \cdot f^{w,2}_{bio,MeHg} \cdot A_w - R_{sw} \cdot f^{w,2}_{aq,MeHg}\right] \cdot C^w_{MeHg2}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + \left(v_{s,A} \cdot f^{w,2}_{abioHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}\right) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,Hg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + \left(v_{s,A} \cdot f^{w,2}_{abioHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}\right) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - \left(kb_{red} + kb_{meth}\right) V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + \left(v_{s,A} \cdot f^{w,2}_{abioMeHg} + v_{sB} \cdot f^{w,2}_{bio,MeHg}\right) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sed,MeHg} \cdot A_w - \left(kb_{demeth} + kb_{mer}\right) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer (1941), cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix	Inverted Matrix									x=b/A
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	4.733E-07	-1.21E-08	-1.12E-08	-5.12E-09	-1.14E-08	-1.13E-08	-5.59E-09	-1.14E-08	-1.12E-08	-5.60E-09	4.73309E-07
C_HgII_1_T	1.12E+08	-6.29E+07	5.53E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	1.866E-06	-2.70E-08	-4.46E-08	-1.21E-08	-3.96E-08	-4.15E-08	-1.42E-08	-3.96E-08	-4.15E-08	-1.42E-08	1.86633E-06
C_MeHg_1_T	0.00E+00	9.50E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	2.250E-07	-9.85E-10	-1.58E-09	-1.60E-07	-3.49E-09	-3.87E-09	-1.48E-07	-3.49E-09	-3.93E-09	-1.48E-07	2.25039E-07
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	1.423E-06	-2.186E-08	-3.389E-08	-1.365E-08	-1.17E-07	-8.10E-08	-2.14E-08	-1.17E-07	-8.10E-08	-2.15E-08	1.42261E-06
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	8.84E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	7.643E-06	-1.141E-07	-1.824E-07	-6.198E-08	-4.04E-07	-4.48E-07	-8.80E-08	-4.04E-07	-4.47E-07	-8.83E-08	7.64329E-06
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	8.84E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T	3.973E-07	-3.187E-09	-5.096E-09	-1.859E-07	-1.13E-08	-1.25E-08	-4.79E-07	-1.13E-08	-1.27E-08	-4.78E-07	3.97302E-07
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	1.181E-06	-1.81E-08	-2.81E-08	-1.13E-08	-9.70E-08	-6.73E-08	-1.78E-08	-4.02E-06	-6.72E-08	-1.78E-08	1.18076E-06
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.27E+08	0.00E+00	0.00E+00	-4.29E+03	3.98E+00	0.00E+00	C_HgII_1_sed	2.256E-01	-3.37E-03	-5.38E-03	-1.83E-03	-1.19E-02	-1.32E-02	-2.60E-03	-1.19E-02	-1.34E-02	-2.61E-03	0.225578848
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.99E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	5.578E-04	-5.19E-06	-8.30E-06	-2.13E-04	-1.84E-05	-2.04E-05	-5.48E-04	-1.84E-05	-2.07E-05	-7.80E-04	0.000557807

A*x=b

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.005
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.000
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		0.062
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.000
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		0.099
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.000
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		0.794
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		0.396
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.000
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.000
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.000
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.000
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		0.049
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		0.025
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.000
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		0.538
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		0.159
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		1.00E+00
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		1.32E-05
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		1.13E-04
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00E+00
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		1.00E+00
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		1.00E+00
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v,HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v,MeHg	water column volatilization loss rate constant, MeHg	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4,792.63
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65E+00
θ sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.030
V_sed	Volume of Sediment	Aw*z_sed m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 2	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

Conversion for Sediment Concentrations
Model Calculates as g Hg per cubic meter (water or sediment particles)

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$kw_{v,i} = \frac{K_{v,i}\cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{wet}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{water}(\theta_{sed})+\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left\{\left[\frac{g\ water}{cm^3\ water}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]+\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3\ water}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]\right\}}$$

$$R_{sw} = \frac{E_{sw}\cdot A_w\cdot\theta_{sed}}{z_{sed}}\cdot 3.1536\text{x}10^7$$

$$K_{eff,i}^{j} = \frac{\left(S_{abio}^{j}C_{abio,i}^{j}+S_{org}^{j}C_{org,i}^{j}+S_{phyto}^{j}C_{phyto,i}^{j}+S_{zoo}^{j}C_{zoo,i}^{j}\right)}{S_{abio}^{j}+S_{org}^{j}+S_{phyto}^{j}+S_{zoo}^{j}} \quad \frac{\left(C_{unfiltered,i}^{j}-C_{filtered,i}^{j}\right)}{C_{diss,i}^{j}+C_{DOC,i}^{j}} = \frac{TSS}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	1.56E-05	15.61
C_HgII_1_Aq			g/m3	2.97E-06	2.97
C_MeHg_1_Aq			g/m3	1.01E-06	1.01
C_Hg0_2_Aq			g/m3	1.10E-04	110.40
C_HgII_2_Aq			g/m3	2.44E-04	243.91
C_MeHg_2_Aq			g/m3	1.47E-05	14.72
C_Hg0_pore			g/m3	1.10E-04	110.40
C_HgII_pore			g/m3	2.91E-04	290.64
C_MeHg_pore			g/m3	3.88E-06	3.88
C_HgT_1_filtered			g/m3	1.96E-05	19.59
C_HgT_2_filtered			g/m3	3.69E-04	369.04
C_HgT_Sed_filtered			g/m3	4.05E-04	404.93
C_Hg0_1_T			g/m3	1.56E-05	15.61
C_HgII_1_T			g/m3	5.77E-05	57.70
C_MeHg_1_T			g/m3	5.52E-06	5.52
C_Hg0_2_T			g/m3	1.10E-04	110.40
C_HgII_2_T			g/m3	6.10E-04	609.66
C_MeHg_2_T			g/m3	1.75E-05	17.52
C_Hg0_sed			g/m3	9.16E-05	91.64
C_HgII_1_sed			g/m3	1.83E+01	18306812.78
C_MeHg_1_sed			g/m3	2.84E-02	28445.58
C_Hg0_sed, wet			g/g	3.46E-11	0.000
C_HgII_1_sed, wet			g/g	1.43E-05	14.297
C_MeHg_1_sed, wet			g/g	3.41E-08	0.034
C_HgT_sed,wet			g/g	1.43E-05	14.331
C_Hg0_sed, dry weight			g/g	2.03E-10	0.00
C_HgII_1_sed, dry weight			g/g	4.06E-05	40.64
C_MeHg_1_sed, dry weight			g/g	6.31E-08	0.06
C_HgT_1			g/m3	7.88E-05	78.82
C_HgT_2			g/m3	7.38E-04	737.58
C_HgT_Sed			g/g	4.07E-05	40.70
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		7.00%	73.20%	19.80%
Layer 2			2.37%	82.66%	14.97%
Sediments			0.16%	99.84%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0.49	
z2	depth of second water layer		m	0.10	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.88548%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	3.06930%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	6.87088%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	4.27053%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	15.22372%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	33.13706%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1	0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1	0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1	0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2	0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2	6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2	0.02796%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red,1} \cdot V_w\right] \cdot C^w_{Hg1l} + \left[kw_{mer} \cdot V_w + kw_{photored} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{1A} \cdot f^{w,1}_{abioHg0} \cdot A_w - v_{1B} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{Hg1l}}{dt} = L_{T,Hg1l} + Q_{in}C_{in,Hg1l} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg1l} V_w - kw_{red1} \cdot V_w - kw_{metlR} \cdot V_w - v_{1A} \cdot f^{w,1}_{abiHg1l} A_w - v_{1B} \cdot f^{w,1}_{bioHg1l} A_w\right] \cdot C^w_{Hg1l} + Q' \cdot C^w_{Hg1l2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{metlB} \cdot V_w\right] \cdot C^w_{Hg1l} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photored} V_w - v_{1A} \cdot f^{w,1}_{abioMeHg} A_w - v_{1B} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{Hg1l2} + \left[kw_{mer} V_w + kw_{photored} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{2A} \cdot f^{w,2}_{abioHg0} \cdot A_w - v_{2B} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0}\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{Hg1l2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demeth} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{metlR} \cdot V_w - v_{2A} \cdot f^{w,2}_{abiHg1l} A_w - v_{2B} \cdot f^{w,2}_{bioHg1l} A_w - R_{sw} \cdot f^{w,2}_{aqHg1l}\right] \cdot C^w_{Hg1l2} + Q' \cdot C^w_{Hg1l} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg1l}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg1l} A_w\right] \cdot C^{sed}_{aqHg1l}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{metlB} \cdot V_w\right] \cdot C^w_{Hg1l2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} V_w - kw_{photored} V_w - v_{2A} \cdot f^{w,2}_{abioMeHg} A_w - v_{2B} \cdot f^{w,2}_{bioMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \cdot \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{2A} \cdot f^{w,2}_{abioHg0} + v_{2B} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{2A} \cdot f^{w,2}_{abioHgII} + v_{2B} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{2A} \cdot f^{w,2}_{abioMeHg} + v_{2B} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)} \qquad E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

A*x=b

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b	
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T
C_HgII_1_T	1.12E+08	-6.29E+07	5.53E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T
C_MeHg_1_T	0.00E+00	9.50E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.57E-01	C_MeHg_1_T
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	8.84E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	8.84E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.83E+01	C_HgII_1_sed
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.99E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed

Solution Matrix	Inverted Matrix										x=b/A
1.561E-05	-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.36E-07	-2.77E-09	1.56E-05	
5.770E-05	-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.77E-09	5.77E-05	
5.517E-06	-1.28E-16	-4.85E-16	-1.59E-07	9.98E-15	-6.81E-16	-1.47E-07	1.16E-12	2.92E-07	-1.47E-07	5.52E-06	
1.104E-04	-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.50E-09	-4.51E-08	6.02E-06	-1.11E-09	0.00011	
6.097E-04	-1.979E-09	-3.165E-09	5.926E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.32E-05	2.43E-08	0.00061	
1.752E-05	1.087E-16	-6.871E-16	-1.840E-07	3.24E-14	-2.18E-15	-4.76E-07	3.74E-12	9.45E-07	-4.75E-07	1.75E-05	
9.164E-05	-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.19E-10	9.16E-05	
1.831E+01	1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.43E-04	3.95E-06	9.98E-01	7.74E-04	18.30681	
2.845E-02	7.24E-13	-2.32E-13	-2.10E-04	5.42E-11	-1.95E-12	-5.43E-04	6.09E-09	1.54E-03	-7.74E-04	0.028446	

C_T_sed 18.33535 g/m3

$$C^{sed}_{dry}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C^{bulk}_{sed}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6 \frac{cm^3}{m^3}\right]}$$

f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1		4.94622%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1		2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2		53.83330%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T_Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T_HgII	Total Load, HgII	g/yr	2.17E+01
L_T_MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v_Hg0	water column volatilization loss rate constant, Hg0	per yr	388.36
kw_v_HgII	water column volatilization loss rate constant, HgII	per yr	0.00
kw_v_MeHg	water column volatilization loss rate constant, MeHg	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant, layer 2	per yr	246.95
kw_red_2	water column reduction rate constant, layer 2	per yr	107.40
kw_meth_1	water column methylation rate constant, layer 1	per yr	0.00
kw_meth_2	water column methylation rate constant, layer 2	per yr	0.00
kw_demeth_1	water column demethylation rate constant, layer 1	per yr	0.00
kw_demeth_2	water column demethylation rate constant, layer 2	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for layer 1	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for layer 2	per yr	6.43
kw_mer	water column *mer* cleavage demethylation rate constant	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation rate constant	per yr	0.00

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-n)}$$

v_sA	abiotic settling velocity	m/yr		4792.628412
v_sB	biotic settling velocity	m/yr		73
v_rs	resuspension velocity	m/yr		0.003700005
k_mort	phytoplankton mortality rate	per yr		10.95
v_min	mineralization rate	per yr		0.01
v_bur	burial rate	m/yr		0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0		m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII		m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg		m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0		m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII		m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg		m2/sec	6.11E-10
rho_s	Sediment Particle Density		g/cm3	2.65E+00
θ_sed	sediment porosity		cm3/cm3	0.83
z_sed	sediment layer,char mixing length		m	0.03
V_sed	Volume of Sediment	Aw*z_sed	m3	11351.43
TSS_1			mg/L	7.90
TSS+2			mg/L	0.56
Effective Partition Coefficients for each Hg species and layer				
K_eff_Hg0_1	Effective K for Hg0 in layer 1		L/kg	0.00E+00
K_eff_Hg0_1	Effective K for Hg0 in layer 2		L/kg	2.33E+06
K_eff_MeHg_1	Effective K for HgII in layer 1		L/kg	5.66E+05
K_eff_Hg0_2	Effective K for HgII in layer 2		L/kg	0.00E+00
K_eff_HgII_2	Effective K for MeHg in layer 1		L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2		L/kg	3.37E+05

$$K_{eff,i}^{j} = \frac{\frac{\left(S_{abio,i}^{j} C_{abio,i}^{j} + S_{org,i}^{j} C_{org,i}^{j} + S_{phyto,i}^{j} C_{phyto,i}^{j} + S_{zoo,i}^{j} C_{zoo,i}^{j}\right)}{S_{abio}^{j} + S_{org}^{j} + S_{phyto}^{j} + S_{zoo}^{j}}}{C_{diss,i}^{j} + C_{DOC,i}^{j}} = \frac{\frac{\left(C_{unfiltered,i}^{j} - C_{filtered,i}^{j}\right)}{TSS}}{C_{filtered,i}^{j}}$$

Water Body Mercury Concentrations

Symbol	Parameter	Equation	Units	Value	Conc. in ng/L : ug/g
C_Hg0_1_Aq			g/m3	6.51E-06	6.51
C_HgII_1_Aq			g/m3	1.24E-06	1.24
C_MeHg_1_Aq			g/m3	4.27E-07	0.43
C_Hg0_2_Aq			g/m3	4.49E-05	44.90
C_HgII_2_Aq			g/m3	9.91E-05	99.14
C_MeHg_2_Aq			g/m3	6.08E-06	6.08
C_Hg0_pore			g/m3	4.49E-05	44.90
C_HgII_pore			g/m3	1.18E-04	118.10
C_MeHg_pore			g/m3	1.60E-06	1.60
C_HgT_1_filtered			g/m3	8.18E-06	8.18
C_HgT_2_filtered			g/m3	1.50E-04	150.12
C_HgT_Sed_filtered			g/m3	1.65E-04	164.59
C_Hg0_1_T			g/m3	6.51E-06	6.51
C_HgII_1_T			g/m3	2.41E-05	24.14
C_MeHg_1_T			g/m3	2.34E-06	2.34
C_Hg0_2_T			g/m3	4.49E-05	44.90
C_HgII_2_T			g/m3	2.48E-04	247.81
C_MeHg_2_T			g/m3	7.23E-06	7.23
C_Hg0_sed			g/m3	3.73E-05	37.27
C_HgII_1_sed			g/m3	7.44E+00	7,438,849.17
C_MeHg_1_sed			g/m3	1.17E-02	11,683.27
C_Hg0_sed, wet			g/g	1.41E-11	0.00
C_HgII_1_sed, wet			g/g	5.81E-06	5.81
C_MeHg_1_sed, wet			g/g	1.40E-08	0.01
C_HgT_sed,wet			g/g	5.82E-06	5.82
C_Hg0_sed, dry weight			g/g	8.27E-11	0.00
C_HgII_1_sed, dry weight			g/g	1.65E-05	16.51
C_MeHg_1_sed, dry weight			g/g	2.59E-08	0.03
C_HgT_1			g/m3	3.30E-05	32.99
C_HgT_2			g/m3	3.00E-04	299.94
C_HgT_Sed, dry weight			g/g	1.65E-05	16.54
			% MeHg	%HgII	% Hg0
Layer 1	(%Me MeHg_T/Hg_T)		7.08%	73.18%	19.74%
Layer 2			2.41%	82.62%	14.97%
Sediments			0.16%	99.84%	0.00%
Q'	Bulk Exchange Flow		m3/yr	3,017,619	
Qin	Inflow		m3/yr	3,474,314	
Qout	Outflow		m3/yr	3,474,314	
Aw	Surface Area of the Water Body		m2	378,381	
E	Exchange rate		m2/yr	2	
V_1	Volume of Layer 1	Aw*z_1	m3	183,741	
V_2	Volume of Layer 2	Aw*z_2	m3	37,838	
z1	depth of first water layer		m	0	
z2	depth of second water layer		m	0	

f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1	100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1	0.88548%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1	3.06930%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2	100.00000%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2	6.87088%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2	14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1	0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of HgII in water column, layer 1	4.27053%
f_DOC_HgII_w_1	DOC complexed fraction of MeHg in water column, layer 1	15.22372%
f_DOC_HgII_w_2	DOC complexed fraction of Hg0 in water column, layer 2	0.00000%
f_DOC_MeHg_w_1	DOC complexed fraction of HgII in water column, layer 2	33.13706%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2	69.96409%

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_1 + z_2)}$$

Q' Bulk exchange flow [L3/T]

Equations for Total Mercury Concentrations of given species (i.e., total Hg0: sorbed + dissolved)

$$V_w \frac{dC^w_{Hg0,1}}{dt} = L_{T,Hg0} + Q_{in}C_{in,Hg0} + \left[kw_{red1} \cdot V_w\right] \cdot C^w_{HgII1} + \left[kw_{mer} \cdot V_w + kw_{photoredW} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHg0} \cdot V_w - kw_{oxid} \cdot V_w - v_{s1} \cdot f^{w,1}_{abiaHg0} \cdot A_w - v_{sB} \cdot f^{w,1}_{bioHg0} \cdot A_w\right] \cdot C^w_{Hg0,1} + Q' \cdot C^w_{Hg0,2}$$

$$V_w \frac{dC^w_{HgII1}}{dt} = L_{T,HgII} + Q_{in}C_{in,HgII} + \left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,1} + \left[kw_{demeth} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q_{out} - Q' - kw_{volHgII} V_w - kw_{red1} \cdot V_w - kw_{methR} \cdot V_w - v_{s1} \cdot f^{w,1}_{abiaHgII} A_w - v_{sB} \cdot f^{w,1}_{bioHgII} A_w\right] \cdot C^w_{HgII1} + Q' \cdot C^w_{HgII2}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = L_{T,MeHg} + Q_{in}C_{in,MeHg} + \left[kw_{methR} \cdot V_w\right] \cdot C^w_{HgII1} + \left[-Q_{out} - Q' - kw_{volMeHg} V_w - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoredd} V_w - v_{s1} \cdot f^{w,1}_{abiaMeHg} A_w - v_{sB} \cdot f^{w,1}_{bioMeHg} A_w\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg}$$

$$V_w \frac{dC^w_{Hg0,2}}{dt} = +\left[kw_{red2} \cdot V_w\right] \cdot C^w_{HgII2} + \left[kw_{mer} V_w + kw_{photoredd} V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{oxid} V_w - v_{s1} \cdot f^{w,2}_{abiHg0} \cdot A_w - v_{sB} \cdot f^{w,2}_{bioHg0} \cdot A_w - R_{sw} \cdot f^{w,2}_{aqHg0}\right] \cdot C^w_{Hg0,2} + Q' \cdot C^w_{Hg0,1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHg0}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w\right] \cdot C^{sed}_{aqHg0}$$

$$V_w \frac{dC^w_{HgII2}}{dt} = +\left[kw_{oxid} V_w\right] \cdot C^w_{Hg0,2} + \left[kw_{demethR} \cdot V_w\right] \cdot C^w_{MeHg} + \left[-Q' - kw_{red2} \cdot V_w - kw_{methR} \cdot V_w - v_{s1} \cdot f^{w,2}_{abiHgII} A_w - v_{sB} \cdot f^{w,2}_{bioHgII} A_w - R_{sw} \cdot f^{w,2}_{aqHgII}\right] \cdot C^w_{HgII2} + Q' \cdot C^w_{HgII1} + \left[R_{sw} \cdot \frac{f^{sed}_{aqHgII}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} A_w\right] \cdot C^{sed}_{aqHgII}$$

$$V_w \frac{dC^w_{MeHg}}{dt} = +\left[kw_{methR} \cdot V_w\right] \cdot C^w_{HgII2} + \left[-Q' - kw_{demeth} \cdot V_w - kw_{mer} \cdot V_w - kw_{photoredd} \cdot V_w - v_{s1} \cdot f^{w,2}_{abiaMeHg} A_w - v_{sB} \cdot f^{w,2}_{biaMeHg} A_w - R_{sw} \cdot f^{w,2}_{aqMeHg}\right] \cdot C^w_{MeHg} + Q' \cdot C^w_{MeHg} + \left[R_{sw} \frac{f^{sed}_{aqMeHg}}{\theta_{sed}} + (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} A_w\right] \cdot C^{sed}_{aqMeHg}$$

$$V_b \frac{dC^{sed}_{Hg0}}{dt} = \left[R_{sw} f^{w,2}_{aqHg0} + (v_{s1} \cdot f^{w,2}_{abiaHg0} + v_{sB} \cdot f^{w,2}_{bioHg0}) \cdot A_w\right] \cdot C^w_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHg0}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHg0} \cdot A_w - kb_{oxid} \cdot V_{sed}\right] C^{sed}_{Hg0} + \left[kb_{red} \cdot V_b\right] \cdot C^{sed}_{HgII} + \left[kb_{mer} \cdot V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{HgII}}{dt} = \left[R_{sw} f^{w,2}_{aqHgII} + (v_{s1} \cdot f^{w,2}_{abiHgII} + v_{sB} \cdot f^{w,2}_{bioHgII}) \cdot A_w\right] \cdot C^w_{HgII} + \left[kb_{oxid} V_{sed}\right] \cdot C^{sed}_{Hg0} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqHgII}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedHgII} \cdot A_w - (kb_{red} + kb_{meth}) \cdot V_{sed}\right] C^{sed}_{HgII} + \left[kb_{demeth} V_{sed}\right] \cdot C^{sed}_{MeHg}$$

$$V_b \frac{dC^{sed}_{MeHg}}{dt} = \left[R_{sw} f^{w,2}_{aqMeHg} + (v_{s1} \cdot f^{w,2}_{abiaMeHg} + v_{sB} \cdot f^{w,2}_{bioMeHg}) \cdot A_w\right] \cdot C^w_{MeHg} + \left[kb_{meth} \cdot V_{sed}\right] \cdot C^{sed}_{HgII} + \left[-R_{sw} \cdot \left(\frac{f^{sed}_{aqMeHg}}{\theta_{sed}}\right) - (v_{rs} + v_b) \cdot f^{sed}_{sedMeHg} \cdot A_w - (kb_{demeth} + kb_{mer}) \cdot V_{sed}\right] C^{sed}_{MeHg}$$

$$Q' = \frac{E_{12} \cdot A_{12}}{0.5 \cdot (z_2 + z_1)}$$

$$E_z = 0.0142 \cdot Z^{1.49} \cdot 365 d/yr$$

where Z is mean total depth (i.e., z1 + z2)
from Mortimer, cited in Schnoor, 1996, pg. 57.
for rivers, this will be different (see Schnoor)

Matrix A	C_Hg0_1_T 1	C_HgII_1_T 2	C_MeHg_1_T 3	C_Hg0_2_T 4	C_HgII_2_T 5	C_MeHg_2_T 6	C_Hg0_1_sed 7	C_HgII_1_sed 8	C_MeHg_1_sed 9	Matrix b		Solution Matrix	Inverted Matrix								x=b/A
C_Hg0_1_T	-1.90E+08	4.54E+07	2.39E+06	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.99E-01	C_Hg0_1_T	6.510E-06	-9.25E-09	-6.71E-09	-3.41E-09	-1.39E-09	-1.94E-10	-2.97E-09	-1.38E-09	8.36E-07	-2.77E-09	6.51E-06
C_HgII_1_T	1.12E+08	-6.29E+07	5.53E-02	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-4.13E+01	C_HgII_1_T	2.414E-05	-1.66E-08	-2.80E-08	-5.80E-09	-2.81E-09	-7.17E-10	-4.49E-09	-2.79E-09	3.08E-06	-3.77E-09	2.41E-05
C_MeHg_1_T	0.00E+00	9.50E-02	-9.76E+06	0.00E+00	0.00E+00	3.02E+06	0.00E+00	0.00E+00	0.00E+00	-9.97E-01	C_MeHg_1_T	2.336E-06	-1.28E-16	-4.85E-16	-1.59E-07	9.98E-15	-6.81E-16	-1.47E-07	1.16E-12	2.92E-07	-1.47E-07	2.34E-06
C_Hg0_2_T	3.018E+06	0.000E+00	0.000E+00	-2.31E+07	4.06E+06	2.43E+05	2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_2_T	4.490E-05	-1.569E-09	-1.446E-09	-1.353E-09	-4.51E-08	-1.40E-09	-2.50E-09	-4.51E-08	6.02E-06	-1.11E-09	4.49E-05
C_HgII_2_T	0.000E+00	1.408E+07	0.000E+00	1.99E+07	-1.34E+08	8.84E-01	0.00E+00	4.29E+03	0.00E+00	0.00E+00	C_HgII_2_T	2.478E-04	-1.979E-09	-3.165E-09	5.926E-09	-7.00E-09	-7.77E-09	1.66E-08	-6.87E-09	3.32E-05	2.43E-08	0.000248
C_MeHg_2_T	0.000E+00	0.000E+00	3.773E+06	0.00E+00	8.84E-01	-8.19E+06	0.00E+00	0.00E+00	4.31E+03	0.00E+00	C_MeHg_2_T	7.226E-06	1.087E-16	-6.871E-16	-1.840E-07	3.24E-14	-2.18E-15	-4.76E-07	3.74E-12	9.45E-07	-4.75E-07	7.23E-06
C_Hg0_sed	0.00E+00	0.00E+00	0.00E+00	2.12E+05	0.00E+00	0.00E+00	-2.55E+05	0.00E+00	0.00E+00	0.00E+00	C_Hg0_sed	3.727E-05	-1.30E-09	-1.20E-09	-1.12E-09	-3.74E-08	-1.16E-09	-2.08E-09	-3.96E-06	4.99E-06	-9.19E-10	3.73E-05
C_HgII_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00	7.45E+00	C_HgII_1_sed	7.439E+00	1.30E-09	1.20E-09	2.10E-04	3.74E-08	1.17E-09	5.43E-04	3.95E-06	9.98E-01	7.74E-04	7.438849
C_MeHg_1_sed	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.93E+06	0.00E+00	1.99E+00	-4.31E+03	0.00E+00	C_MeHg_1_sed	1.168E-02	7.24E-13	-2.32E-13	-2.10E-04	5.42E-11	-1.95E-12	-5.43E-04	6.09E-09	1.54E-03	-7.74E-04	0.011683

A*x=b

Target C_sed, wet 7.450569701 g/g

f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1		0.53471%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1		0.00410%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2		6.15876%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2		0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1		9.92923%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1		79.43383%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1		39.61797%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2		0.00000%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2		0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1		0.00000%
f_org_HgII_w_1	orqanic particulate phase fraction of HqII in water column, layer 1		4.94622%
f_org_MeHg_w_1	orqanic particulate phase fraction of MeHq in water column, layer 1		2.46695%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2		0.00000%
f_org_HgII_w_2	orqanic particulate phase fraction of HqII in water column, layer 2		53.83330%
f_org_MeHg_w_2	orqanic particulate phase fraction of MeHq in water column, layer 2		15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments		100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments		0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments		0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments		0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments		99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments		99.98867%
L_T,Hg0	Total Load, Hg0	g/yr	3.99E-01
L_T,HgII	Total Load, HgII	g/yr	2.17E+01
L_T,MeHg	Total Load, MeHg	g/yr	7.43E-01
Rate Constants			
kw_v,Hg0	water column volatiilization loss rate cc	per yr	388.36
kw_v,HgII	water column volatiilization loss rate cc	per yr	0.00
kw_v,MeHg	water column volatiilization loss rate cc	per yr	0.65
kw_oxid_1	water column oxidation rate constant	per yr	610.22
kw_oxid_2	water column oxidation rate constant	per yr	525.60
kw_red_1	water column reduction rate constant,	per yr	246.95
kw_red_2	water column reduction rate constant,	per yr	107.40
kw_meth_1	water column methylation rate constar	per yr	0.00
kw_meth_2	water column methylation rate constar	per yr	0.00
kw_demeth_1	water column demethylation rate cons	per yr	0.00
kw_demeth_2	water column demethylation rate cons	per yr	0.00
kw_photodegrad_1	water column photoreduction rate for I	per yr	13.03
kw_photodegrad_2	water column photoreduction rate for I	per yr	6.43
kw_mer	water column *mer* cleavage demethyl	per yr	0.00
kb_oxid	benthic oxidation rate constant	per yr	0.00
kb_red	benthic reduction rate constant	per yr	0.00
kb_methy	benthic methylation rate constant	per yr	0.00
kb_demeth	benthic demethylation rate constant	per yr	0.00
kb_mer	benthic *mer* cleavage demethylation r	per yr	0.00
v_sA	abiotic settling velocity	m/yr	4792.628412
v_sB	biotic settling velocity	m/yr	73
v_rs	resuspension velocity	m/yr	0.003700005
k_mort	phytoplankton mortality rate	per yr	10.95
v_min	mineralization rate	per yr	0.01
v_bur	burial rate	m/yr	0.007620015
R_sw_Hg0	pore water diffusive volume, Hg0	m3/yr	2.12E+05
R_sw_HgII	pore water diffusive volume, HgII	m3/yr	2.12E+05
R_sw_MeHg	pore water diffusive volume, MeHg	m3/yr	2.02E+05
E_sw_Hg0	pore water diffusion coefficient,Hg0	m2/sec	6.41E-10
E_sw_HgII	pore water diffusion coefficient, HgII	m2/sec	6.41E-10
E_sw_MeHg	pore water diffusion coefficient, MeHg	m2/sec	6.11E-10
rho_s	Sediment Particle Density	g/cm3	2.65
θ_sed	sediment porosity	cm3/cm3	0.83
z_sed	sediment layer,char mixing length	m	0.03
V_sed	Volume of Sediment Aw*z_sed	m3	11351.43
TSS_1		mg/L	7.90
TSS+2		mg/L	0.56
Effective Partition Coefficients for each Hg species and layer			
K_eff_Hg0_1	Effective K for Hg0 in layer 1	L/kg	0.00E+00
K_eff_HgII_1	Effective K for HgII in layer 1	L/kg	2.33E+06
K_eff_MeHg_1	Effective K for MeHg in layer 1	L/kg	5.66E+05
K_eff_Hg0_2	Effective K for Hg0 in layer 2	L/kg	0.00E+00
K_eff_HgII_2	Effective K for HgII in layer 2	L/kg	2.67E+06
K_eff_MeHg_2	Effective K for MeHg in layer 2	L/kg	3.37E+05

$$kw_{v,i} = \frac{K_{v,i} \cdot f_{aq,i}^{w,1}}{z_1}$$

$$\frac{[Hg(OH)_2][H^+]^2}{[Hg^{2+}]} = 10^{-6.2}$$

$$C_{dry}^{sed}\left[\frac{g\ Hg}{g\ sed}\right] = \frac{C_{sed}^{bulk}}{\rho_{particle}(1-\theta_{sed})} = \frac{\left[\frac{g\ Hg}{m^3\ bulk}\right]}{\left[\frac{g\ sed}{cm^3\ sed}\right]\left[\frac{m^3}{m^3\ bulk}\right]\left[10^6\frac{cm^3}{m^3}\right]}$$

$$R_{sw} = \frac{E_{sw} \cdot A_w \cdot \theta_{sed}}{z_{sed}} \cdot 3.1536 \text{x} 10^7$$

$$K_{eff,i}^j = \frac{\left(S_{abio}^j C_{abio,i}^j + S_{org}^j C_{org,i}^j + S_{phyto}^j C_{phyto,i}^j + S_{zoo}^j C_{zoo,i}^j\right)}{S_{abio}^j + S_{org}^j + S_{phyto}^j + S_{zoo}^j} = \frac{\left(C_{unfiltered,i}^j - C_{filtered,i}^j\right)}{TSS}$$
$$\frac{}{C_{diss,i}^j + C_{DOC,i}^j} \qquad \frac{}{C_{filtered,i}^j}$$

Mercury Loading to Water Body

$$L_{T,i} = L_{Dep,i} + L_{RI,i} + L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{R,i} + L_{E,i} + L_{Diff,i}$$

Symbol	Parameter	Equation	Units	Value
L_T,Hg0	Total Load, Hg0		g/yr	0.40
L_T,HgII	Total Load, HgII		g/yr	21.72
L_T,MeHg	Total Load, MeHg		g/yr	0.74

Direct Deposition Load

$$L_{Dep,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_w$$

Symbol	Parameter	Equation	Units	Value
L_Dep,Hg0	Deposition Loading, Hg0	Flux*Area	g/yr	**0.00E+00**
L_Dep,HgII	Deposition Loading, HgII	Flux*Area	g/yr	**7.32**
L_Dep,MeHg	Deposition Loading, MeHg	Flux*Area	g/yr	**0.116465672**
Net Flux, Hg0		D_wet+D_dry	ug/m2-yr	0
Net Flux, HgII		D_wet+D_dry	ug/m2-yr	19.34
Net Flux, MeHg		D_wet+D_dry	ug/m2-yr	0.3078

Wet and Dry Deposition

$$D_{wet,i} = C_{precip,i} \bullet P$$

D_dry,Hg0	Dry Deposition Flux, Hg0	ug/m2-yr	0	User
D_dry,HgII	Dry Deposition Flux, HgII	ug/m2-yr	10	User
D_dry,MeHg	Dry Deposition Flux, MeHg	ug/m2-yr	0.15	User
D_wet,Hg0	Wet Deposition Flux, Hg0	ug/m2-yr	0	User
D_wet,HgII	Wet Deposition Flux, HgII	ug/m2-yr	9.34	User
D_wet,MeHg	Wet Deposition Flux, MeHg	ug/m2-yr	0.1578	User
C_Precip,Hg0	Conc in Precip, Hg0	ug/m3	0	
C_Precip,HgII	Conc in Precip, HgII	ug/m3	10	
C_Precip, MeHg	Conc in Precip, MeHg	ug/m3	0.15	1.5% wet
P	Average Annual Precipitation Rate	cm/yr	105.2	

Impervious Surface Runoff Load

$$L_{RI,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,I} \bullet R_{I,i}$$

Symbol	Parameter	Equation	Units	Value
L_RI,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RI,HgII	Impervious Runoff, HgII		g/yr	**0.26**
L_RI,MeHg	Impervious Runoff, MeHg		g/yr	**0.00**

Wetland Runoff Load

$$L_{RW,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,W} \bullet R_{W,i}$$

Symbol	Parameter	Equation	Units	Value
L_RW,Hg0	Wetland Runoff, Hg0		g/yr	**0.00**
L_RW,HgII	Wetland Runoff, HgII		g/yr	**1.33**
L_RW,MeHg	Wetland Runoff, MeHg		g/yr	**0.52**

Riparian Runoff Load

$$L_{RR,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,R} \bullet R_{L,i}$$

Symbol	Parameter	Equation	Units	Value
L_RR,Hg0	Riparian Runoff, Hg0		g/yr	**0.00**
L_RR,HgII	Riparian Runoff, HgII		g/yr	**0.33**
L_RR,MeHg	Riparian Runoff, MeHg		g/yr	**0.05**

Upland Runoff Load

$$L_{RU,i} = \left(D_{dry,i} + D_{wet,i}\right) \bullet A_{C,U} \bullet R_{U,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**0.39**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.01**

Contaminated Soils Runoff Load

$$L_{CW,i} = ks_{RO,i} \bullet A_{C,C} \bullet z_S \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_RU,Hg0	Impervious Runoff, Hg0		g/yr	**0.00**
L_RU,HgII	Impervious Runoff, HgII		g/yr	**11.40**
L_RU,MeHg	Impervious Runoff, MeHg		g/yr	**0.04**

Pervious Surface Runoff Load

$$L_{R,i} = L_{RW,i} + L_{RR,i} + L_{RU,i} + L_{CW,i}$$

Symbol	Parameter	Equation	Units	Value
L_R,Hg0	Pervious Runoff, Hg0		g/yr	**0.00**
L_R,HgII	Pervious Runoff, HgII		g/yr	**13.47**
L_R,MeHg	Pervious Runoff, MeHg		g/yr	**0.62**

Soil Erosion Load

$$L_{E,i} = ks_{e,i} \bullet V_s \bullet C_{s,i}$$

Symbol	Parameter	Equation	Units	Value
L_E,Hg0	Erosion load, Hg0		g/yr	**0**
L_E,HgII	Erosion load, HgII		g/yr	**0**
L_E,MeHg	Erosion load, MeHg		g/yr	**0**

Gaseous Diffusion Load (Volatilization)

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Load, Hg0		g/yr	**0.40**
L_Diff,HgII	Gaseous Diffusion Load, HgII		g/yr	**0.67**
L_Diff,MeHg	Gaseous Diffusion Load, MeHg		g/yr	**0.00**

Gaseous Diffusion Loading

Symbol	Parameter	Equation	Units	Value
L_Diff,Hg0	Gaseous Diffusion Loading, Hg0		g/yr	3.99E-01
L_Diff,HgII	Gaseous Diffusion Loading, HgII		g/yr	6.73E-01
L_Diff,MeHg	Gaseous Diffusion Loading, MeHg		g/yr	6.15E-04
C_a,Hg0	Gaseous Concentration of Hg0		ug/m3	1.60E-03
C_a,HgII	Gaseous Concentration of HgII		ug/m3	3.00E-06
C_a,MeHg	Gaseous Concentration of MeHg		ug/m3	3.00E-09

$$L_{Dif,i} = K_{v,i} \bullet A_w \bullet \left(\frac{C_{a,i} \cdot 10^{-6}}{\frac{H_i}{RT}} \right)$$

Mason, R.P., W.F. Fitzgerald, F.M.M.Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic Influences. Geochimica et Cosmochimica Act. 58(15): 3191-1918 states that the atmosphere has an average concentration of 1.6 ng/m3 = 0.0016 ug/m3 and that 98% of this is Hg0

Symbol	Parameter	Equation	Units	Value
K_v,Hg0,T	overall transfer rate, Hg0, adj for T		m/yr	1.89E+02
K_v,HgII,T	overall transfer rate, HgII, adj for T		m/yr	1.69E-02
K_v,MeHg,T	overall transfer rate, MeHg, adj for T		m/yr	1.03E+01
Theta	T correction factor		--	1.026
H,Hg0	Henry's Law Constant, Hg0		atm-m3/mole	7.10E-03
H,HgII	Henry's Law Constant, HgII		atm-m3/mole	7.10E-10
H,MeHg	Henry's Law Constant, MeHg		atm-m3/mole	4.70E-07
R	Universal Gas Constant		atm-m3/mole-K	8.21E-05
T	water body temperature		Kelvin	302.54
Aw	Surface area of the waterbody		m2	3.78E+05

Overall transfer rate, K_v,i

$$K_{v,i} = \left(R_{L,i} + R_{G,i}\right)^{-1} = \left({K_{L,i}}^{-1} + \left(K_{G,i} \frac{H_i}{RT_K} \right)^{-1} \right)^{-1}$$

Symbol	Parameter	Equation	Units	Value
K_v,Hg0	overall transfer rate, Hg0		m/yr	1.89E+02
K_v,HgII	overall transfer rate, HgII		m/yr	1.70E-02
K_v,MeHg	overall transfer rate, MeHg		m/yr	1.03E+01
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05

Liquid transfer coefficient, K_L,i

$$K_{L,i} = u \bullet \left(\frac{\rho_a}{\rho_w} \right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2} \right) Sc_{w,i}^{-0.67} \left(3.15 x 10^{7} \right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_L,Hg0	liquid phase transfer coefficient,Hg0		m/yr	1.89E+02
K_L,HgII	liquid phase transfer coefficient,HgII		m/yr	1.89E+02
K_L,MeHg	liquid phase transfer coefficient,MeHg		m/yr	1.83E+02
Sc_w,Hg0	Schmidt number for water, Hg0		--	2.98E+03
Sc_w,HgII	Schmidt number for water, HgII		--	2.98E+03
Sc_w,MeHg	Schmidt number for water, MeHg		--	3.12E+03
Tw	Temperature of reference water (T=20)		C	20
μw	viscosity of water		g/cm-s	0.019049

$$Sc_{w,i} = \frac{\mu_w}{\rho_w D_{w,i}}$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.155(T_w - 20) + 0.00585(T_w - 20)^2} \right] - 3.0233$$

Gas transfer coefficient, K_G,i

$$K_{G,i} = u \bullet \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_{a,i}^{-0.67} \left(3.15x10^{7}\right)$$

Calculated for T = 20 C (293.15 K)

Symbol	Parameter	Equation	Units	Value
K_G, Hg0	gas phase transfer coefficient, Hg0		m/yr	5.94E+05
K_G, HgII	gas phase transfer coefficient, HgII		m/yr	5.94E+05
K_G, MeHg	gas phase transfer coefficient, MeHg		m/yr	5.75E+05
Sc_a,Hg0	Schmidt number for air, Hg0		--	2.71E+00
Sc_a,HgII	Schmidt number for air, HgII		--	2.71E+00
Sc_a,MeHg	Schmidt number for air, MeHg		--	2.84E+00

$$Sc_{a,i} = \frac{v_a}{D_{a,i}}$$

Parameters used in calculations of transfer coefficients

u	shear velocity	u=sqrt(Cd)*W	m/s	0.198997
Cd	drag coefficient		--	0.0011
W	wind velocity, 10 m above water surface		m/s	6
ρa	density of air		g/cm3	1.20E-03
ρw	density of water		g/cm3	0.99824
k	von Karman's constant			0.4
λ2	viscous sublayer thickness			4
va	dynamic viscosity of air		cm2/sec	0.14991
Ta	air temperature		C	19.9

$$u^* = C_d^{0.5} W$$

density 1.204 kg/m3 at 20 C [if we want to change with T, we'll need formula]

$$\rho_w = 1 - 8.8x10^{-5} T_w$$

$$v_a = (1.32 + 0.009 \bullet T_a)x10^{-1}$$

Divalent Mercury Speciation

Predominant Mercury Species Present

	log K	alphas layer 1	layer 2	Sediment
Hg^{++}	--	7.94E-09	7.94E-09	7.94E-09
$HgCl_2$	13.2	9.02E-06	9.02E-06	9.02E-06
$Hg(OH)_2$	21.8	1.00E+00	1.00E+00	1.00E+00
$Hg(SO_4)_2$	1.34	9.05E-15	9.05E-15	9.05E-15
HgS	-53	2.48E-75	2.48E-75	2.48E-75

		layer 1	layer 2	Sediment
Cl^-	Moles/L	8.46E-06	8.46E-06	8.46E-06
SO_4^{2-}	Moles/L	5.21E-08	5.21E-08	5.21E-08
S^{2-}	Moles/L	3.12E-14	3.12E-14	3.12E-14
OH^-	Moles/L	1.41E-07	1.41E-07	1.41E-07
pH	--	7.15	7.15	7.15

$$[Hg^{++}] = \alpha_0 C_{T,Hg^{++}}$$

$$\alpha_0 = \frac{1}{1 + K_{HgCl}[Cl^-]^2 + K_{Hg(OH)_2}[OH^-]^2 + K_{HgSO_4}[SO_4^{2-}] + K_{HgS}[S^{2-}]}$$

$$\alpha_1 = K_{HgCl}[Cl^-]^2 \alpha_0$$

$$\alpha_2 = K_{Hg(OH)_2}[OH^-]^2 \alpha_0$$

$$\alpha_3 = K_{HgSO_4}[SO_4^{2-}] \alpha_0$$

$$\alpha_4 = K_{HgS}[S^{2-}] \alpha_0$$

Concentrations

		layer 1	layer 2	Sediment
Cl^-	mg/L	0.3	0.3	0.3
SO_4^{2-}	mg/L	5.0E-03	5.0E-03	5.0E-03
S^{2-}	mg/L	1.0E-09	1.0E-09	1.0E-09

Assumption

Cl^- = Total Chloride
SO_4^{2-} = Total Sulfate
S^{2-} = Total Sulfide

Molecular Weights

Cl^-	amu	35.45	35.45	35.45
SO_4^{2-}	amu	96.056	96.056	96.056
S^{2-}	amu	32.06	32.06	32.06

Equilibrium Partitioning

Symbol	Parameter	Equation	Units	Value
f_aq_Hg0_w_1	aqueous phase fraction of Hg0 in water column, layer 1			100.00000%
f_aq_Hg0_w_2	aqueous phase fraction of Hg0 in water column, layer 2			100.00000%
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.88548%
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87088%
f_aq_MeHg_w_1	aqueous phase fraction of MeHg in water column, layer 1			3.06930%
f_aq_MeHg_w_2	aqueous phase fraction of MeHg in water column, layer 2			14.10566%
f_DOC_Hg0_w_1	DOC complexed fraction of Hg0 in water column, layer 1			0.00000%
f_DOC_Hg0_w_2	DOC complexed fraction of Hg0 in water column, layer 2			0.00000%
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27053%
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			33.13706%
f_DOC_MeHg_w_1	DOC complexed fraction of MeHg in water column, layer 1			15.22372%
f_DOC_MeHg_w_2	DOC complexed fraction of MeHg in water column, layer 2			69.96409%
f_abio_Hg0_w_1	abiotic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_abio_Hg0_w_2	abiotic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_abio_HgII_w_1	abiotic particulate phase fraction of HgII in water column, layer 1			0.53471%
f_abio_HgII_w_2	abiotic particulate phase fraction of HgII in water column, layer 2			6.15876%
f_abio_MeHg_w_1	abiotic particulate phase fraction of MeHg in water column, layer 1			0.00410%
f_abio_MeHg_w_2	abiotic particulate phase fraction of MeHg in water column, layer 2			0.02796%
f_zoo_Hg0_w_1	zooplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_zoo_Hg0_w_2	zooplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_zoo_HgII_w_1	zooplankton particulate phase fraction of HgII in water column, layer 1			9.92923%
f_zoo_HgII_w_2	zooplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_zoo_MeHg_w_1	zooplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_zoo_MeHg_w_2	zooplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_phyto_Hg0_w_1	phytoplankton particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_phyto_Hg0_w_2	phytoplankton particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_phyto_HgII_w_1	phytoplankton particulate phase fraction of HgII in water column, layer 1			79.43383%
f_phyto_HgII_w_2	phytoplankton particulate phase fraction of HgII in water column, layer 2			0.00000%
f_phyto_MeHg_w_1	phytoplankton particulate phase fraction of MeHg in water column, layer 1			39.61797%
f_phyto_MeHg_w_2	phytoplankton particulate phase fraction of MeHg in water column, layer 2			0.00000%
f_org_Hg0_w_1	organic particulate phase fraction of Hg0 in water column, layer 1			0.00000%
f_org_Hg0_w_2	organic particulate phase fraction of Hg0 in water column, layer 2			0.00000%
f_org_HgII_w_1	organic particulate phase fraction of HgII in water column, layer 1			4.94622%
f_org_HgII_w_2	organic particulate phase fraction of HgII in water column, layer 2			53.83330%
f_org_MeHg_w_1	organic particulate phase fraction of MeHg in water column, layer 1			2.46695%
f_org_MeHg_w_2	organic particulate phase fraction of MeHg in water column, layer 2			15.90229%
f_aq_Hg0_sed	aqueous phase fraction of Hg0 in sediments			100.00000%
f_aq_HgII_sed	aqueous phase fraction of HgII in sediments			0.00132%
f_aq_MeHg_sed	aqueous phase fraction of MeHg in sediments			0.01133%
f_sed_Hg0_sed	particulate phase fraction of Hg0 in sediments			0.00000%
f_sed_HgII_sed	particulate phase fraction of HgII in sediments			99.99868%
f_sed_MeHg_sed	particulate phase fraction of MeHg in sediments			99.98867%
Sbio_phyto,1	Concentration of Phytoplankton, Layer 1		g/m3	5 from 'Solids Balance'
Sbio_zoo,1	Concentration of Zooplankton, Layer 1		g/m3	2.5
Sbio_phyto,2	Concentration of Phytoplankton, Layer 2		g/m3	0
Sbio_zoo,2	Concentration of Zooplankton, Layer 2		g/m3	0
Sabio_1	Concentration of suspended inorganic particles, Layer 1		g/m3	0.08
Sabio_2	Concentration of suspended inorganic particles, Layer 2		g/m3	0.12
Sbio_dead,1	Concentration of non-living (dead) particles, Layer 1		g/m3	0.31
Sbio_dead,2	Concentration of non-living (dead) particles, Layer 2		g/m3	0.44
S_abio, sed	Concentration of inorganic particles in sediment		g/m3	52,833.08
S_bio_dead,sed	Concentration of non-living (dead) particles in sediment		g/m3	2,743.46
DOC_1	Dissolved Organic Carbon Concentration in Layer 1		g/m3	16
DOC_2	Dissolved Organic Carbon Concentration in Layer 2		g/m3	16

$$f_{aq,i}^{w,j} = \frac{1}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)}$$

$$f_{abio,i}^{w,j} = \frac{K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{abio,i}^{aq}\cdot S_{abio}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{DOC,i}^{w,j} = \frac{K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}}{1+10^{-6}\left(K_{abio,i}^{aq}\cdot S_{abio}\cdot + K_{bio\_zoo,i}^{aq}\cdot S_{bio,zoo} + K_{bio\_phyto,i}^{aq}\cdot S_{bio,phyto} + K_{bio\_dead,i}^{aq}\cdot S_{bio,dead} + K_{DOC,i}\cdot S_{DOC}\right)} = K_{DOC,i}^{aq}\cdot S_{DOC}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{zoo,i}^{w,j} = K_{zoo,i}^{aq}\cdot S_{zoo}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{phyto,i}^{w,j} = K_{phyto,i}^{aq}\cdot S_{phyto}^{w,j}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{org,i}^{w,j} = K_{org,i}^{aq}\cdot S_{org}\cdot 10^{-6}\cdot f_{aq,i}^{w,j}$$

$$f_{aq,i}^{sed} = \frac{\theta_{sed}}{\theta_{sed} + K_{abio,i}^{sed}\cdot S_{abio,i}^{sed}\cdot 10^{-6} + K_{bio\_dead,i}^{sed}\cdot S_{bio\_dead,i}^{sed}\cdot 10^{-6}}$$

$$f_{sed,i}^{sed} = 1 - f_{aq,i}^{sed}$$

Symbol	Parameter	Units	Value	
K_aq_abio_Hg0	partition coefficient for Hg0 to abiotic solids	L/kg	0	
K_aq_abio_HgII	partition coefficient for HgII to abiotic solids	L/kg	7,182,936	
K_aq_abio_MeHg	partition coefficient for MeHg to abiotic solids	L/kg	15,887	
K_aq_phyto_Hg0	partition coefficient for Hg0 to phytoplankton	L/kg	0	
K_aq_phyto_HgII	partition coefficient for HgII to phytoplankton	L/kg	17,941,378	
K_aq_phyto_MeHg	partition coefficient for MeHg to phytoplankton	L/kg	2,581,565	
K_aq_zoo_Hg0	partition coefficient for Hg0 to zooplankton	L/kg	0	
K_aq_zoo_HgII	partition coefficient for HgII to zooplankton	L/kg	4,485,345	assumed to be 0.25* phytoplankton
K_aq_zoo_MeHg	partition coefficient for MeHg to zooplankton	L/kg	5,163,130	assumed to be 2 * phytoplankton
K_aq_org_Hg0	partition coefficient for Hg0 to dead biomass	L/kg	0	assumed the same as phytoplankton
K_aq_org_HgII	partition coefficient for HgII to dead biomass	L/kg	17,941,378	assumed the same as phytoplankton
K_aq_org_MeHg	partition coefficient for MeHg to dead biomass	L/kg	2,581,565	assumed the same as phytoplankton
K_DOC_Hg0	partition coefficient for Hg0 to DOC	L/kg	0	
K_DOC_HgII	partition coefficient for HgII to DOC	L/kg	301,427	
K_DOC_MeHg	partition coefficient for MeHg to DOC	L/kg	310,000	
K_B_Hg0	partition coefficient for Hg0 to benthic solids	L/kg	0	
K_B_HgII	partition coefficient for HgII to benthic solids	L/kg	260,558	
K_B_MeHg	partition coefficient for MeHg to benthic solids	L/kg	4,557	
θ_B	sediment porosity	L/L	0.83	

Solids Balance

	g/m3				
Sbio_phyto,1	5		TSS_1	7.90	mg/L
Sbio_zoo,1	2.5		TSS_2	0.56	mg/L
Sbio_phyto,2	0				
Sbio_zoo,2	0				
Sabio_1	8.41E-02				
Sabio_2	1.25E-01				
Sbio_dead,1	3.11E-01				
Sbio_dead,2	4.37E-01				
S_abio, sed	5.28E+04				
S_bio_dead,sed	2.74E+03				
S_sed,total	5.56E+04	g/m3			

Parameters for Solids Balance

Symbol	Parameter	Units	Value		Notes
A_w	Surface Area of Water Body	m2	3.78E+05	Link	
A_c	Surface Area of Catchment	m2	6.48E+05	Link	
Q_in	Water Inflow	m3/yr	3.47E+06	Link	
Q_out	Water Outflow	m3/yr	3.47E+06	Link	
Sabio_in	Abiotic solids in water inflow	g/m3	44	User	
Sbio_phyto,in	Phytoplankton biotic solids in water inflow	g/m3	0.95	User	
Sbio_zoo,in	Zooplankton biotic solids in water inflow	g/m3	5	User	
Sbio_phyto,1	Phytoplankton Conc. in layer 1	g/m3	5	Model	1
Sbio,zoo,1	Zooplankton Conc. in layer 1	g/m3	2.5	Model	2
Sbio_phyto,2	Phytoplankton Conc. in layer 2	g/m3	0	set to 0	3
Sbio,zoo,2	Zooplankton Conc. in layer 2	g/m3	0	set to 0	3
rho_s	sediment density	g/cm3	2.65	assumed default (range: 2 - 2.7)	
θ_sed	Sediment porosity	cm3/cm3	0.83		
d_s	sediment particle diameter	um	13	Default: mid-silt	4,6
v_sA	abiotic settling velocity	m/day	1.31E+01	Modeled	
v_sB	biotic settling velocity	m/day	0.2	Default	7
v_rs_abio	resuspension velocity, abiotic	m/day	0.000010137	Default	9
v_rs_bio_dead	resuspension velocity,dead biotic	m/day			5
k_mort_1	phytoplankton mortality rate in layer 1	per day	0.03	Default	8
k_mort_2	phytoplankton mortality rate in layer 2	per yr			
v_sA	abiotic settling velocity	m/yr	4792.628	Link	
v_sB	biotic settling velocity	m/yr	73	Link	
v_rs	resuspension velocity	m/yr	3.70E-03	Link	
k_mort	phytoplankton mortality rate	per yr	10.95	Link	
d_sed	Depth of sediment layer	m	0.03	default	
v_min	mineralization rate	per yr	0.01	mid of R-MCM	
A=	R*K*LS*C	kg/m2-yr	0.202	RUSLE Result	10
LSE	watershed solids erosion load	kg/m2-yr	0.000	Adjusted for loss	11
z1	Layer 1 water depth	m	0.485598171	Link	
z2	Layer 2 water depth	m	0.1	Link	
E12	Exchange Rate between layers	m2/yr	2.335096212	currently no exchange	
A12	interfacial area of epi/hyp	m	378381	(currently set to Aw)	
Q'	Bulk Exchange Flow	m3/yr	3017618.85	modeled as 0	
Vw_1	Volume of Layer 1	m3	183741.1216	Link	
Vw_2	Volume of Layer 2	m3	37838.1	Link	
LSB	net internal production rate of biota	g/m2-yr	912.5	Model	5
v_b	burial velocity	m/yr	0.007620015	0.3in/year 0.3 in/39.37 in/meter = 0.01 m/y	
Theta_sed	Sediment porosity	--	0.83	default	

Revised Universal Soil Loss Equation

Part of the Country	Eastern (1) or West (2)		1	East
A		kg/m2/yr	0.2016	
R	Soil Erosivity Factor	kg/km2-yr (tons/acre)/	200	12
K	Soil Erodibility Factor	(kg/km2)	0.3	
LS	Topographic Factor	--	2.5	
C	Cover Management Factor	--	0.006	

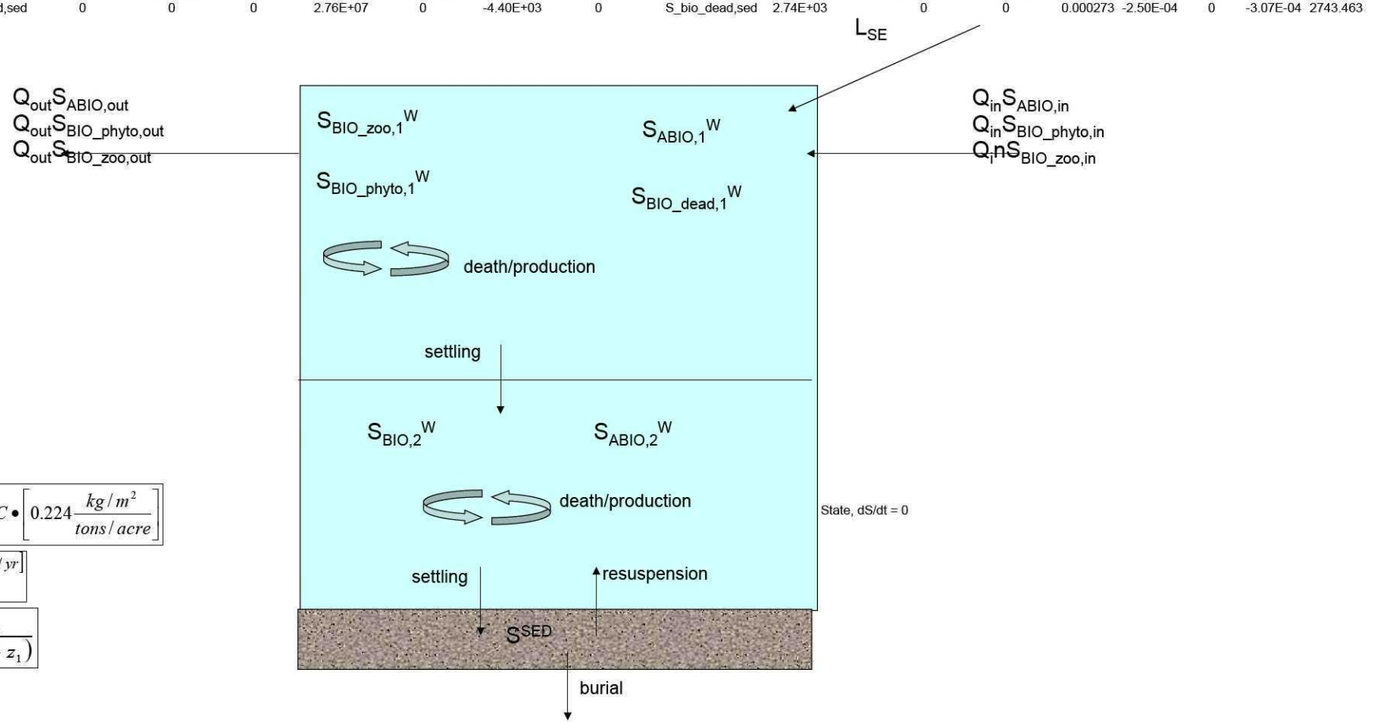
$$A = R \bullet K \bullet LS \bullet C \bullet \left[0.224 \frac{kg/m^2}{tons/acre}\right]$$

$$L_{SE} = S_{del} \bullet A\left[kg/m^2/yr\right]$$

$$S_{del} = 1.26 \bullet A_C^{-0.125}$$

$$Q' = \frac{E_{12} A_{12}}{0.5 \cdot (z_2 + z_1)}$$

Matrix A	S_abio,1	S_abio,2	S_bio_dead,1	S_bio_dead,2	S_abio,sed	S_bio_dead,sed		Solution Matrix	Matrix Inversion						x=b/A
	1	2	3	4	5	6	b								
S_abio,1	1.81E+09	3.02E+06	0	0	0	0	1.53E+08	S_abio,1	8.41E-02	5.50E-10	1.36E-12	0	0	4.43E-13	0	0.084069
S_abio,2	1.82E+09	-1.82E+09	0	0	1400.01159	0	0	S_abio,2	1.25E-01	8.16E-10	-8.15E-10	0	0	-2.7E-10	0	0.12479
S_bio_dead,1	0	0	2.81E+07	3.02E+06	0	0	1.01E+07	S_bio_dead,1	3.11E-01	0	0	3.09E-08	4.28E-09	0	1.36E-09	0.311342
S_bio_dead,2	0	0	3.06E+07	-3.06E+07	0	1.40E+03	0	S_bio_dead,2	4.37E-01	0	0	4.34E-08	-3.98E-08	0	-1.27E-08	0.4367
S_abio,sed	0	1.81E+09	0	0	-4.28E+03	0	0	S_abio,sed	5.28E+04	0.000346	-3.45E-04	0	0	-3.46E-04	0	52833.08
S_bio_dead,sed	0	0	0	2.76E+07	0	-4.40E+03	0	S_bio_dead,sed	2.74E+03	0	0	0.000273	-2.50E-04	0	-3.07E-04	2743.463



$$V_1 \frac{dS^w_{abio,1}}{dt} = +\left[L_{SE} \cdot A_c \cdot 10^3\right] + Q_{in} S_{abio,in} - Q_{out} S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,1}$$

$$V_2 \frac{dS^w_{abio,2}}{dt} = +v_{sA} \cdot A_w \cdot S^w_{abio,1} - v_{sA} \cdot A_w \cdot S^w_{abio,2} + v_{rs} \cdot A_w \cdot S^{sed}_{abio}$$

		Oligo	Meso	Eutro	Dystro
1	Modeled from Wetzel.				
	Wetzel (mg C/m3)	20-100	100-300	>300	<50-200
	Used (mg C/m3)	60	200	500	125
	Used (g/m3)	0.12	0.4	1	0.25

assumed 2 g phytoplankton per 1 g C.

2 Assumed one half as much zooplankton as phytoplankon (need to check on this)
3 currently assume all zooplankton and phytoplankton are in upper layer
4 User should enter the mean particle size diameter.
This is an area where a more refined approach could be used using particle distributions.
Sands should not be included in the distribution, because they will tend to settle immediately and not resuspend.
See below for typical ranges of particles
Modeling at steady-state, the mortality rate is equal to the negative of the growth rate.
mortality is modeled as first order, and productivity is a flux, so divide productivity by phyto concentration and thickness of layer.

		50-300	250-1000	>1000	<50-500
5	Modeled from Wetzel				
	Wetzel (mg C/m2/day)				
	Used (mg C/m2/day)	175	625	1250	275
	Used (g/m2/yr)	127.75	456.25	912.5	200.75

6 Particle Size Distributions

		Size Range (um)
Silt	Coarse	62 - 31
	Medium	31 - 16
	Fine	16 - 8
	Very Fine	8-4
Clay	Coarse	4-2
	Medium	2-1
	Fine	1-0.5
	Very Fine	0.5-0.24

7 From Mercury Report to Congress, 1997. citiing Bowie, et al, 1985, settling is 0.02 - 2 m/day, 0.2 was used.
8 From Mercury Report to Congress, 1997. citing Bowie, et al., 1985, range from 0.003 to 0.17 per day
9 From Mercury Report to Congress, 1997. estimate resuspension as 0.0037 m/yr 1.0137E-05 m/day
10 Soil Erosion from Mercury Report to Congress, 1997. Default 200 kg/km2/yr for Western locations default 53 kg/m2/yr
11 Sediment Delivery Ratio to Water Body
12 200 is the mid-range Eastern value, but decreases in the north and increases in the south
In Alabama and Mississippi, values reach in to the 400s, while in Michigan they fall below 100.

$$V_1 \frac{dS^w_{bio\_dead1}}{dt} = +k_{mort} \cdot S^w_{bio\_phyto1} \cdot V_1 - v_{sB} \cdot A_w \cdot S^w_{bio\_dead1}$$

$$V_2 \frac{dS^w_{bio\_dead2}}{dt} = +k_{mort} S_{bio\_phyto2} V_2 + v_{sB} \cdot A_w \cdot S^w_{bio\_dead1} - v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} + v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead}$$

$$V_{sed} \frac{dS^{sed}_{abio}}{dt} = v_{sA} \cdot A_w \cdot S^w_{abio2} - v_{rs} \cdot A_w \cdot S^{sed}_{abio} - v_b \cdot A_w \cdot S^{sed}_{abio}$$

$$V_{sed} \frac{dS^{sed}_{bio\_dead}}{dt} = v_{sB} \cdot A_w \cdot S^w_{bio\_dead2} - v_{rs} \cdot A_w \cdot S^{sed}_{bio\_dead} - v_{\min} \cdot V_{sed} \cdot S^{sed}_{bio\_dead} - v_b \cdot A_w \cdot S^{sed}_{bio\_dead}$$

Kinetic Rate Constants

Water column Abiotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_1	abiotic methylation in layer 1		per day	0.00000016	1	2
k_meth_2	abiotic* methylation in layer 2		per day	0.0000016	1	4
k_meth_1	abiotic methylation in layer 1		per yr	0.0000584		
k_meth_2	abiotic* methylation in layer 2		per yr	0.000584		
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			0.00885	3	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			0.06871		
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			0.04271		
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			0.33137		
k_meth_1	abiotic methylation in layer 1		per yr	5.17E-07		
k_meth_2	abiotic* methylation in layer 2		per yr	2.34E-05	if anoxic:	

$$k_{meth} = k_{meth,base} * f_{HgII}^{aq}$$

$$k_{meth} = k_{meth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC}\right)$$

Notes

1 Mercury Report to Congress
2 Value used is the same as the one used in the Mercury Report to Congress. This is a mid-range value in a range of 0.0001 - 0.003 per day as reported in Gilmour and Henry, 1991. Ranges of values are presented in the Methylation in Water Column table.
3 According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions
4 If the hypolimnion is anoxic, then methylation occurs in the hypolimnion at a rate of 0.01 per day. The * denotes that biotic methylation is occuring if there is anoxia

Sediment Biotic Methylation of HgII => MeHg

Symbol	Parameter	Equation	Units	Value	Notes	
k_meth_b	biotic methylation in sediments		per day	0.00000048	1	2
k_meth_b	biotic methylation in sediments		per yr	0.0001752		

Notes

1 Mercury Report to Congress presents 0.0001 per day
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present methylation of new HgII as 0.012 - 0.016/d, while old mercury is 0.001/day

Water column Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes
k_demeth_1	biotic demethylation in layer 1		per day	0.000000016	1
k_demeth_2	biotic demethylation in layer 2		per day	0.00000016	
k_demeth_1	biotic demethylation in layer 1		per yr	0.00000584	
k_demeth_2	biotic demethylation in layer 2		per yr	0.0000584	
f_aq_HgII_w_1	aqueous phase fraction of HgII in water column, layer 1			8.85E-03	
f_aq_HgII_w_2	aqueous phase fraction of HgII in water column, layer 2			6.87E-02	
f_DOC_HgII_w_1	DOC complexed fraction of HgII in water column, layer 1			4.27E-02	
f_DOC_HgII_w_2	DOC complexed fraction of HgII in water column, layer 2			3.31E-01	
k_demeth_1	biotic demethylation in layer 1		per yr	3.01E-07	
k_demeth_2	biotic demethylation in layer 2		per yr	2.34E-05	

$$k_{demeth} = k_{demeth\ ,base} * \left(f_{HgII}^{aq} + f_{HgII}^{DOC}\right)$$

Notes

1 From Matilainen and Verta. 1995. Mercury methylation and demethylation in aerobic surface waters Canadian Journal of Fisheries and Aquatic Sciences. 52:1597-1608. mean rates used. Needs to be investigated for dependencies on DOC, particulates, temperature, color.
According to research done by Matilainen, and Verta, 1995, abiotic methylation was suppressed by color and particulates suggesting that only aqueous dissolved (non-DOC complexed) HgII is the only reacting mercury. Also in this article, DOC increased the rate of biotic demethylation suggesting that biotic reactions can happen to both DOC-complexed and aqueous. Therefore, these reactions are multiplied by the associated fractions

Sediment Biotic Demethylation of MeHg => HgII

Symbol	Parameter	Equation	Units	Value	Notes	
k_demeth_b	biotic demethylation in sediments		per day	0.00000096	1	2
k_demeth_b	biotic demethylation in sediments		per yr	0.0003504		

Notes

1 Mercury Report to Congress
2 from Hintelmann, H., K. Keppel-Jones, R. D. Evans. 2000. Constants of Mercury Methylation and Demethylation Rates in Sediments and Comparison of Tracer and Ambient Mercury Availability. Environ. Tox. Chem. 19(9): 2204-2211.
present demethylation of new HgII as 0.416 - 0.528/d, while old mercury is 0.390/day

Reduction of HgII (Biotic): HgII -> Hg0

Symbol	Parameter	Equation	Units	Value	Notes	
kw_basered	base reduction rate		per day	0.03	2	
kw_basered_sed	base reduction rate in sediments		per day	0		* currently assume no reduction in sediments
alpha_red_1	ratio of Hg(OH)2 to HgII, layer 1		--	1.00	3	
alpha_red_2	ratio of Hg(OH)2 to HgII, layer 2		--	1.00		
alpha_red_sed	ratio of Hg(OH)2 to HgII, sed		--	1.00		
kw_red_1	abiotic reduction in layer 1		per day	3.00E-02		
kw_red_2	abiotic reduction in layer 2		per day	3.00E-02		
kb_red	abiotic reduction in sediment		per day	0.00E+00		
kw_red_1	abiotic reduction in layer 1		per yr	10.95		
kw_red_2	abiotic reduction in layer 2		per yr	10.95		
kb_red	abiotic reduction in sediment		per yr	0.00		

Notes

1 Chlorine Conc assumed to be 0.3 mg/L (from R-MCM) need to research this, or have user enter reasonable value.
2 Value of 0.03/day is used in R-MCM, this needs to be researched for a more supportable value
Value of 0.03/day is taken from Mason, R.P., F.M.M. Morel, H.F.Hemond. 1995. The Role of Microorganisms in Elemental Mercury Formation in Natural Waters. Water, Air, and Soil Pollution. **80**: 775-787.
Mean lake value of 2% to 4% per day. This rate varies over the year, possibly along with microorganism activity.
Only mercury in the form of [Hg(OH)2] can be reduced from HgII to HgO
For most surface water bodies, Hg(OH)2 (dissolved) is the dominant mercury species, this
is a function of pH and redox potential,
for more reduced waters, Hg0 will dominate, in more reduced and acidic water, HgCl2 will dominate. This should be further researched.
3 Speciation of mercury is calculated in "Speciation" spreadsheet and linked here

Photo-Degradation (MeHg -> Hg0)

k_photored_base	base photoreduction rate constant	per day per E/m2-day	0.002	1
k_photored_1	MeHg photored rate constant 1	per day	3.57E-02	
k_photored_2	MeHg photored rate constant 2	per day	1.76E-02	
k_photored_1	MeHg photored rate constant 1	per year	1.30E+01	
k_photored_2	MeHg photored rate constant 2	per year	6.43E+00	

Notes

1 From Sellers, P., C.A. Kelly, J.W.M. Rudd, A.R. MacHutchon. 1996. Photodegradation of Methylmercury in Lakes. Nature. 380(25). April
From Fig. 2a. k=0.0022*PAR
From Fig. 2b. k=0.0019*PAR Value used: 0.002*PAR PAR = E/m2-day

Photo-Reduction (HgII -> Hg0)

k_photo_vis,study	rate for vis = 21 W/m2	per hr	1	1	1
k_photo_UV-B,study	rate for UV-B = 0.4 W/m2	per hr	1.2	1	1.2
k_photoreduct_base_vis	base photoreduction rate constant, vis	per hour per uE/m2-sec	0.0010	calculated for comparison to input	
k_photoreduct_base_vis	base photoreduction rate constant, vis	per day per E/m2-day	0.0300		

$$k_{photored\_i} = k_{photored\_base} * \overline{E}$$

k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per hour per uE/m2-sec	0.10	calculated for comparison to input
k_photoreduct_base_UV-B	base photoreduction rate constant, UV-B	per day per E/m2-day	28.25	
k_photoreduct_avg_1,vis	Avg rate over layer 1, vis	per day	0.54	
k_photoreduct_avg_2,vis	Avg rate over layer 2, vis	per day	0.26	
k_photoreduct_avg_1,UV-B	Avg rate over layer 1, UV-B	per day	0.11	
k_photoreduct_avg_2,UV-B	Avg rate over layer 1, UV-B	per day	0.00	
k_photoreduct_1	sum of vis + UV-B	per day	0.65	
k_photoreduct_2	sum of vis + UV-B	per day	0.26	
k_photoreduct_1	sum of vis + UV-B	per yr	236.00	
k_photoreduct_2	sum of vis + UV-B	per yr	96.45	

Notes

1 from Amyot, M. D.R.S. Lean, L. Poissant, M-R Doyon. 2000. Distribution and Transformation of Elemental Mercury in the St. Lawrence River and Lake Ontario. Can. J. Aquat. Sci. 57 (Suppl. 1): 155-163.
Photoreduction rates presented as dependent on both vis and UV-B. For UV-B + vis, k = 2.2 +/- 0.2 per hr. For vis only, k = 1.0 +/- 0.1 per hour. Assume, k = 1.2 +/- 0.1 per hour for UV-B alone
The intensity of incident light for these experiments was vis = 21 W/m2, and UV-B 0.4 W/m2.
Converting to uE/m2/sec, vis = 103.57 uE/m2/s, UV-B = 1.03 uE/m2/s
This is the calculation as given by Amyot, 2000. In LaLonde, et al, 2001, it states that the work done here was done at 10 times the incident UV radiation as presented in LaLonde et al., 2001.
The UV-B is presented there as 1.18 uE/m2/s, therefore 11.8 uE/m2/s is used for UV-B, and
The rate of photo-reduction is calculated by summing both the rate of vis and UV-B light induced photoreduction
These are done separately first, because UV-B attenuates faster in natural waters than vis.

Photo-Oxidation (Hg0 -> HgII)

k_photo_UV-B, study	rate for UV-B - 1.18 uE/m2/s	per hr	0.25	1
k_photooxid_base	base photooxidation rate constant	per hour per uE/m2/s	0.21	
k_photooxid_base	base photooxidation rate constant	per day per E/m2-day	58.85	
k_oxid	dark oxidation	per day	1.44	2
k_photooxid_avg_1	Avg rate over layer 1	per day	1.67	
k_photooxid_avg_2	Avg rate over layer 2	per day	1.44	
k_photooxid_avg_1	Avg rate over layer 1	per yr	610.22	
k_photooxid_avg_2	Avg rate over layer 2	per yr	525.60	

Notes

1 from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
In freshwater, k = 0.25 +/- 0.02 per hour, w/UV-B = 1.18 uE/m2/s
2 from LaLond, et al, 2001. oxidation occurred at a rate of 0.06 per hr in the dark in a saline water. This is negligible when sunlight is present, but may be significant at lower regions, and is therefore included.

$$k\_photo\_base = \frac{0.25 hr^{-1}}{1.18 uE/m^2/s}$$

$$k\_photo\_oxid = k\_photo\_base \cdot UVB$$

Light Intensity

Symbol	Parameter	Equation	Units	Value	Notes
z_1	Thickness of Layer 1		m	0.485598171	
z_2	Thickness of Layer 2		m	0.1	
Surface Light	Surface Light Intensity: accounting for weath		E/m2-day	29.33	
Surface Light - UV-B	Surface UV-B Intensity		E/m2-day	0.15	
ke	Light Extinction Coefficient		per m	2.25	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
η UV-B extinction coefficient (layer	UV light extinction = f(DOC)		per m	76.66	
E_avg_1	Avg Light over depth of layer 1		E/m2-day	17.84	
E_avg_2	Avg Light over depth of layer 2		E/m2-day	8.81E+00	
UV_avg_1	Avg UV over depth of layer 1		E/m2-day	3.94E-03	
UV_avg_2	Avg UV over depth of layer 2		E/m2-day	1.30E-18	

1 $\overline{E} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_0 e^{-k_e x} dx = \frac{1}{x_2 - x_1}\frac{E_0}{k}\left[e^{-k_e x_1} - e^{-k_e x_2}\right]$

$z_2 = x_2 - x_1$

$\overline{E}_{UV-B} = \frac{1}{x_2 - x_1}\int_{x_1}^{x_2} E_{0,UV} e^{-\eta_{UV-B} x} dx = \frac{1}{x_2 - x_1}\frac{E_{0,UV-B}}{k}\left[e^{-\eta_{UV-B} x_1} - e^{-\eta_{UV-B} x_2}\right]$

$\eta_{UV-B} = 0.4415 * (DOC)^{.86}$

UV-B relation to DOC
from LaLonde, J.D., M. Amyot, A.M.L. Kraepiel, F.M.M.Morel. 2001. Photooxidation of Hg(0) in Artificial and Natural Waters. Environ. Sci. Technol. 35: 1367-1372,
citing *Scully, NM, Lean, DRS. Arch. Hydrobiol. Beih.* **1994.** *43*,135.

1 UV-B is modeled as being 0.5% of visible light.
check?

Net Reduction (Hg0 -> HgII): Photo-Reduction plus Biotic Reduction

Symbol	Parameter	Equation	Units	Value	Notes
kw_red_1	abiotic reduction in layer 1		per yr	10.95	
kw_red_2	abiotic reduction in layer 2		per yr	10.95	
k_photoreduct_1	sum of vis + UV-B		per yr	236.00	
k_photoreduct_2	sum of vis + UV-B		per yr	96.45	
k_net_reduction_1	net rate of reduction		per yr	246.95	
k_net_reduction_2	net rate of reduction		per yr	107.40	

Location		
East		YES
West		NO

Revisions

Version No.	Date	Changes
1.0.1	2/15/2006	Separated Partitioning into sorption to zooplankton, phytoplankton, and organic solids.
		This was done so that only organic matter settles, not phytoplankton or zooplankton
1.0.2	6/6/2006	Updated Aqueous Concentrations to be sum of Dissolved/Non-Complexed and Dissolved/Complexed
		Updated Algorithm for Avg UV Radiation if DOC = 0. If DOC=0, then Avg UV = Incident UV. For hypolimnion, UV = Avg of Layer 1.
		Defined "Effective Partition Coefficient" for each scenario.
1.0.3	4/26/2007	Caught linkage error for demethylation rate constant. Was linking to per day, is fixed to link to per year
1.0.3a	6/14/2007	a-line of SERAFM created to distinguish from parallel b line. In SERAFMa, the model maintains the original functionality of using VBA 6 to solve system of linear equations
		Because VBA 5 does not support the syntax to solve a linear system of equations in this way, SERAFMb was created for version of Excel before Excel 2003 and for Macintosh users.
1.0.3b	6/14/2007	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
"LITE"	6/14/2007	SERAFM-Lite created for each the a and b lines of SERAFM.
		In this version, the contaminated sediment scenarios have been removed to boil SERAFM down to the mercury cycling aquatic ecosystem,
		which can be used as is to investigate mercury concentrations in a given system or adapted to study systems with different loading scenarios.
1.0.4a	8/8/2007	Solids balance error found. Total fractions of f_i_HgII_w_1 were not summing to 1.
		For f_aq_HgII_w_1, link was to Sabio_2 (E59) was fixed to go to Sbio_dead,1 (E60)
		For f_org_HgII_w_1, link was to K_aq_org_MeHg (E80) was fixed to go to K_aq_org_HgII (E79)
Olin Site Specific	1/18/2010	Matrix multiplication uses "MINVERSE" to invert the matrix and "MMULT" to multiply the inv of A by column vector b.
Application of SERAFM		Matrix multiplication originally designed for Mac, incorporated into this version to minimize need for VBA and macros for Excel (minimize divide by 0 error upon opening).
		BAF restructuring: In the original SERAFM, BAFs for wildlife calculations were linked to the Input/output worksheet.
		In this application, BAFs were linked within the wildlife worksheet to include more species for different trophic levels
		The original SERAFM based the target clean-up on dry sediment Hg concentrations, where it should have been using wet sediment concentrations.
		The new SERAFM now uses the wet concentration, and links that value to the Target C_sed_Hg page. This change has resulted in the Target Sensitive Species HI becoming or almost becoming equal to 1 (HI=1).
		The original SERAFM Wildlife Page, cell C3 called the value representing the total dissolved MeHg fraction from the WaterBody C_Sed_Hg page, while this version for Olin calls the filtered
		MeHg from Cell H8 of the input out page. This reflects the use of site specific BAFs that were based on the filtered MeHg measurements

Calculation of Inflow and Outflow

APPENDIX C

SERAFM MODEL INPUTS AND OUTPUTS

The SERAFM model typically uses a hydraulic residence time (input by the user) to calculate inflow and outflow volumes. Water elevations are recorded on a regular basis at OU-2, which allows the inflow and outflow volumes to be calculated from recorded data rather than an assumed residence time. The following section explains the methods used to calculate the inflow and outflow volumes to the Basin.

Basin water elevations have been recorded at the gate by a data logger since July 2009. Elevations were recorded by hand prior to having the data logger and in the case of power or equipment failure at the gate control room. The 2008 and 2009 Basin elevations used to calculate inflow and outflow are shown in Figures C-1 and C-2, respectively. In some cases where data were not available, the water elevations were estimated by using the Leroy River Gauge elevation as a guide.

The difference in water elevation from one data point to the next was calculated for each data point. Positive differences (rise in water elevation) were considered inflows; negative differences (decreasing water elevation) were considered outflows. Each water elevation difference was then multiplied by the surface area of the Basin appropriate for the scenario. The surface area used for Scenario 1 is outlined in purple on Figure C-3 and represents the 6-foot elevation within the berm. The surface area used for Scenarios 2 and 3 is outlined in yellow on Figure C-3 and represents the 3-foot elevation within the Basin. These elevations were interpolated by ArcGIS. They were bounded to exclude areas that might be at or below the given elevation, but not within the areas of the Basin controlled by the gate structure.

The incremental inflows and outflows were calculated using the following formula:

$$\Delta Water\ Elevation * Surface\ Area = Incremental\ Inflow\ or\ Outflow$$

Incremental inflows for the year were summed together; incremental outflows for the year were also summed together. The absolute value of the outflow sum was then averaged with the inflow sum using the following formula:

$$Inflow\backslash Outflow = \frac{|yearly\ outflow\ sum| + yearly\ inflow\ sum}{2}$$

This average was used as the inflow/outflow SERAFM input. Individual inflow/outflow inputs were calculated for each year (one input each for 2008 and 2009). The full calculations are provided in Tables C-1 and C-2.

TABLE C-1: 2008 INFLOW/OUTFLOW CALCULATIONS
Olin McIntosh Operable Unit 2, McIntosh, Alabama

Date	Basin Elevation (ft NAVD88)	Elevation Change from Previous Data Point (m)	Surface Area (m^2)	Incremental Outflow Volume (m^3)	Incremental Inflow Volume (m^3)
2/1/2008 12:20	3.4				
2/2/2008 7:16	5.0	0.5	274544	0	134238
2/3/2008 11:18	7.2	0.7	274544	0	186748
2/4/2008 8:01	7.6	0.1	274544	0	30125
2/6/2008 12:12	8.0	0.1	274544	0	36262
2/7/2008 11:21	8.4	0.1	274544	0	34867
2/8/2008 10:30	8.5	0.0	274544	0	8368
2/9/2008 9:55	8.9	0.1	274544	0	33472
2/11/2008 10:27	8.8	0.0	274544	-8368	0
2/12/2008 11:00	8.8	0.0	274544	0	0
2/13/2008 11:22	8.8	0.0	274544	0	0
2/14/2008 9:00	8.4	-0.1	274544	-37656	0
2/16/2008 7:00	7.1	-0.4	274544	-104601	0
2/18/2008 22:20	5.6	-0.5	274544	-125522	0
2/20/2008 13:25	5.3	-0.1	274544	-26778	0
2/21/2008 18:32	5.3	0.0	274544	0	1674
2/23/2008 17:30	8.5	1.0	274544	0	267779
2/24/2008 11:40	10.7	0.7	274544	0	186888
2/29/2008 12:06	11.0	0.1	274544	0	20033
3/7/2008 11:00	11.3	0.1	274544	0	23202
3/10/2008 8:30	13.1	0.6	274544	0	154810
3/11/2008 8:15	12.9	-0.1	274544	-16736	0
3/12/2008 8:15	12.3	-0.2	274544	-50209	0
3/13/2008 8:00	11.6	-0.2	274544	-58577	0
3/14/2008 7:45	11.2	-0.1	274544	-33472	0
3/16/2008 22:00	10.1	-0.3	274544	-92049	0
3/20/2008 11:30	8.4	-0.5	274544	-142258	0
3/25/2008 11:30	6.6	-0.6	274544	-154810	0
3/31/2008 8:00	5.2	-0.4	274544	-112969	0
4/1/2008 14:30	4.8	-0.1	274544	-33472	0
4/2/2008 15:30	4.6	-0.1	274544	-16736	0
4/3/2008 14:00	4.4	-0.1	274544	-16736	0
4/4/2008 8:00	4.9	0.2	274544	0	41841
4/7/2008 12:00	9.4	1.4	274544	0	372380
4/8/2008 8:30	10.3	0.3	274544	0	79497
4/9/2008 9:00	10.7	0.1	274544	0	33472
4/10/2008 8:30	11.0	0.1	274544	0	25104
4/14/2008 8:00	11.0	0.0	274544	0	0
4/15/2008 10:00	10.4	-0.2	274544	-50209	0
4/16/2008 10:00	9.9	-0.2	274544	-41841	0
4/17/2008 10:30	9.4	-0.2	274544	-41841	0
4/18/2008 12:00	8.7	-0.2	274544	-58577	0
4/21/2008 8:00	7.7	-0.3	274544	-83681	0
4/22/2008 7:45	7.1	-0.2	274544	-50209	0

TABLE C-1: 2008 INFLOW/OUTFLOW CALCULATIONS
Olin McIntosh Operable Unit 2, McIntosh, Alabama

Date	Basin Elevation (ft NAVD88)	Elevation Change from Previous Data Point (m)	Surface Area (m^2)	Incremental Outflow Volume (m^3)	Incremental Inflow Volume (m^3)
4/23/2008 15:00	6.2	-0.3	274544	-75313	0
4/25/2008 10:00	5.5	-0.2	274544	-58577	0
4/28/2008 20:00	4.7	-0.2	274544	-66945	0
4/29/2008 7:30	4.2	-0.2	274544	-41841	0
4/30/2008 10:45	3.8	-0.1	274544	-33472	0
5/5/2008 8:00	4.1	0.1	274544	0	25104
5/6/2008 8:00	4.0	0.0	274544	-8368	0
5/19/2008 9:00	11.0	2.1	274544	0	585767
5/20/2008 7:30	11.4	0.1	274544	0	33472
5/21/2008 8:30	11.4	0.0	274544	0	0
5/22/2008 11:00	11.3	0.0	274544	-8368	0
5/23/2008 8:00	11.0	-0.1	274544	-25104	0
5/27/2008 14:30	10.5	-0.2	274544	-41841	0
5/28/2008 7:30	9.5	-0.3	274544	-83681	0
5/29/2008 9:45	8.9	-0.2	274544	-50209	0
5/30/2008 10:00	8.5	-0.1	274544	-33472	0
6/2/2008 7:30	7.0	-0.5	274544	-125522	0
6/3/2008 8:30	6.3	-0.2	274544	-58577	0
6/5/2008 14:30	5.4	-0.3	274544	-75313	0
6/6/2008 12:07	5.1	-0.1	274544	-25104	0
6/9/2008 7:15	4.1	-0.3	274544	-83681	0
6/10/2008 8:30	3.7	-0.1	274544	-33472	0
6/16/2008 9:30	3.7	0.0	274544	0	0
8/25/2008 12:45	4.8	0.3	274544	0	87865
8/26/2008 12:20	6.7	0.6	274544	0	161783
8/27/2008 10:30	8.3	0.5	274544	0	135284
8/28/2008 10:30	8.9	0.2	274544	0	49163
9/2/2008 8:30	8.9	0.0	274544	0	1046
9/3/2008 9:00	8.2	-0.2	274544	-62761	0
9/4/2008 9:30	7.3	-0.3	274544	-71129	0
9/5/2008 13:00	6.4	-0.3	274544	-79497	0
9/8/2008 8:00	4.8	-0.5	274544	-129706	0
9/9/2008 11:00	4.2	-0.2	274544	-51882	0
9/10/2008 13:30	3.6	-0.2	274544	-48535	0
12/10/2008 9:30	2.9	-0.2	274544	-56903	0
12/11/2008 11:00	3.5	0.2	274544	0	50627
12/12/2008 7:30	4.7	0.3	274544	0	94141
12/12/2008 8:20	4.7	0.0	274544	0	0
12/12/2008 10:45	4.7	0.0	274544	0	0
12/12/2008 11:07	4.7	0.0	274544	0	5021
12/12/2008 13:00	4.7	0.0	274544	-837	0
12/13/2008 11:30	9.6	1.5	274544	0	410037
12/15/2008 11:15	13.2	1.1	274544	0	297068
12/17/2008 9:00	15.3	0.7	274544	0	179914

TABLE C-1: 2008 INFLOW/OUTFLOW CALCULATIONS
Olin McIntosh Operable Unit 2, McIntosh, Alabama

Date	Basin Elevation (ft NAVD88)	Elevation Change from Previous Data Point (m)	Surface Area (m^2)	Incremental Outflow Volume (m^3)	Incremental Inflow Volume (m^3)
12/18/2008 9:00	16.0	0.2	274544	0	58577
12/20/2008 11:30	16.1	0.0	274544	0	8368
12/21/2008 14:00	15.7	-0.1	274544	-33472	0
12/22/2008 11:00	15.0	-0.2	274544	-58577	0
12/23/2008 9:00	14.1	-0.3	274544	-75313	0
12/24/2008 11:00	12.9	-0.4	274544	-100417	0
12/25/2008 15:30	11.6	-0.4	274544	-108785	0
12/26/2008 9:15	11.6	0.0	274544	0	0
12/27/2008 8:30	9.9	-0.5	274544	-142258	0
12/28/2008 0:00	9.2	-0.2	274544	-58577	0
12/29/2008 9:50	9.5	0.1	274544	0	25104
12/30/2008 9:15	9.6	0.0	274544	0	8368
12/31/2008 9:15	9.0	-0.2	274544	-50209	0
2008 TOTALS				-3415022	3887471
	Inflow/Outflow = (Outflow sum + |Inflow Sum|) ÷ 2 =				**3,651,247**

Prepared/Date: KPW 05/25/11
Checked/Date: NTG 05/25/11

TABLE C-2: 2009 INFLOW/OUTFLOW CALCULATIONS
Olin McIntosh Operable Unit 2, McIntosh, Alabama

Date	Basin Elevation (ft NAVD88)	Elevation Change from Previous Data Point (m)	Surface Area (m^2)	Incremental Outflow Volume (m^3)	Incremental Inflow Volume (m^3)
1/2/09 8:25	8.3		275681		
1/2/09 10:25	8.3	0.0	275681	0	0
1/5/09 9:00	8.5	0.1	275681	0	16806
1/6/09 10:00	7.7	-0.2	275681	-67222	0
1/7/09 9:00	7.9	0.1	275681	0	16806
1/8/09 10:00	10.6	0.8	275681	0	222673
1/9/09 9:15	12.5	0.6	275681	0	163854
1/10/09 14:30	14.4	0.6	275681	0	159652
1/11/09 14:15	16.0	0.5	275681	0	134444
1/12/09 9:00	17.0	0.3	275681	0	84028
1/13/09 10:45	18.0	0.3	275681	0	84028
1/14/09 10:30	18.5	0.2	275681	0	42014
1/15/09 10:15	18.7	0.1	275681	0	16806
1/16/09 12:20	18.8	0.0	275681	0	8403
1/17/09 12:46	18.6	-0.1	275681	-16806	0
1/18/09 13:36	18.1	-0.2	275681	-42014	0
1/19/09 9:00	17.2	-0.3	275681	-75625	0
1/20/09 8:30	15.6	-0.5	275681	-134444	0
1/21/09 8:30	13.7	-0.6	275681	-159652	0
1/22/09 10:45	11.8	-0.6	275681	-159652	0
1/23/09 13:45	11.2	-0.2	275681	-50417	0
1/24/09 10:00	10.8	-0.1	275681	-33611	0
1/25/09 13:25	10.8	0.0	275681	0	0
1/26/09 10:45	10.8	0.0	275681	0	0
1/26/09 13:45	10.8	0.0	275681	0	0
1/27/09 13:45	10.6	-0.1	275681	-16806	0
1/28/09 13:10	10.2	-0.1	275681	-35292	0
1/29/09 12:10	9.7	-0.1	275681	-40333	0
1/30/09 13:30	9.1	-0.2	275681	-50417	0
2/2/09 13:45	8.1	-0.3	275681	-84028	0
2/3/09 10:30	7.5	-0.2	275681	-50417	0
2/4/09 13:45	6.8	-0.2	275681	-58819	0
2/5/09 13:00	6.4	-0.1	275681	-33611	0
2/6/09 13:30	6.1	-0.1	275681	-25208	0
2/9/09 7:45	5.7	-0.1	275681	-33611	0
2/10/09 10:30	5.7	0.0	275681	-3361	0
2/11/09 13:00	5.7	0.0	275681	-840	0
2/12/09 12:45	5.7	0.0	275681	0	0
2/13/09 14:00	5.7	0.0	275681	0	0
2/16/09 14:30	5.7	0.0	275681	0	0
2/17/09 9:00	5.7	0.0	275681	0	0
2/18/09 10:30	5.7	0.0	275681	0	0

TABLE C-2: 2009 INFLOW/OUTFLOW CALCULATIONS
Olin McIntosh Operable Unit 2, McIntosh, Alabama

Date	Basin Elevation (ft NAVD88)	Elevation Change from Previous Data Point (m)	Surface Area (m^2)	Incremental Outflow Volume (m^3)	Incremental Inflow Volume (m^3)
2/19/09 11:00	5.6	0.0	275681	-4201	0
2/20/09 10:30	5.6	0.0	275681	0	0
2/25/09 9:00	5.5	0.0	275681	-8403	0
2/26/09 11:00	5.5	0.0	275681	0	0
2/27/09 9:30	5.5	0.0	275681	0	0
3/3/09 4:00	10.5	1.5	275681	0	420138
3/10/09 9:45	16.9	2.0	275681	0	537776
3/11/09 15:50	15.7	-0.4	275681	-100833	0
3/12/09 16:00	13.3	-0.7	275681	-201666	0
3/13/09 10:00	11.5	-0.5	275681	-151250	0
3/14/09 13:15	10.8	-0.2	275681	-58819	0
3/15/09 10:30	10.5	-0.1	275681	-25208	0
3/16/09 12:15	10.2	-0.1	275681	-25208	0
3/19/09 12:45	13.7	1.1	275681	0	294096
3/22/09 10:25	16.9	1.0	275681	0	268888
3/23/09 10:15	16.2	-0.2	275681	-58819	0
3/25/09 10:25	13.1	-0.9	275681	-260485	0
4/24/09 13:00	9.4	-1.1	275681	-310902	0
4/27/09 7:30	9.7	0.1	275681	0	25208
4/28/09 8:00	8.7	-0.3	275681	-84028	0
4/29/09 9:30	7.3	-0.4	275681	-117639	0
4/30/09 13:00	6.5	-0.2	275681	-67222	0
5/4/09 11:00	6.4	0.0	275681	-8403	0
5/5/09 7:00	6.4	0.0	275681	0	0
5/5/09 10:30	6.4	0.0	275681	0	0
5/5/09 15:40	9.8	1.0	275681	0	285694
5/6/09 7:25	9.4	-0.1	275681	-33611	0
5/6/09 12:59	9.8	0.1	275681	0	33611
5/7/09 8:20	10.4	0.2	275681	0	53778
5/7/09 15:50	11.1	0.2	275681	0	55458
5/8/09 7:30	11.4	0.1	275681	0	24368
5/8/09 10:12	11.8	0.1	275681	0	34451
5/11/09 13:00	14.6	0.9	275681	0	235277
5/12/09 9:30	15.3	0.2	275681	0	58819
5/14/09 13:30	16.1	0.2	275681	0	67222
5/15/09 10:45	16.0	0.0	275681	-8403	0
5/22/09 0:00	5.7	-3.1	275681	-865484	0
5/29/09 9:35	11.9	1.9	275681	0	520971
6/2/09 9:30	11.3	-0.2	275681	-50417	0
6/3/09 8:12	11.1	0.0	275681	-13444	0
6/3/09 18:30	11.1	0.0	275681	-7562	0
6/4/09 7:55	10.8	-0.1	275681	-21007	0
6/4/09 14:00	10.3	-0.2	275681	-46215	0

TABLE C-2: 2009 INFLOW/OUTFLOW CALCULATIONS
Olin McIntosh Operable Unit 2, McIntosh, Alabama

Date	Basin Elevation (ft NAVD88)	Elevation Change from Previous Data Point (m)	Surface Area (m^2)	Incremental Outflow Volume (m^3)	Incremental Inflow Volume (m^3)
6/5/09 8:00	8.6	-0.5	275681	-138645	0
6/5/09 16:14	8.2	-0.1	275681	-33611	0
6/6/09 9:00	7.6	-0.2	275681	-47055	0
6/6/09 15:50	7.5	0.0	275681	-11764	0
6/7/09 8:30	7.4	0.0	275681	-11764	0
6/7/09 15:26	7.3	0.0	275681	-5882	0
6/8/09 7:55	7.2	0.0	275681	-9243	0
6/8/09 14:38	7.2	0.0	275681	0	1681
6/9/09 7:55	7.1	0.0	275681	-10083	0
6/9/09 14:30	7.0	0.0	275681	-6722	0
6/23/09 7:34	5.7	-0.4	275681	-109236	0
6/23/09 12:15	5.7	0.0	275681	0	0
7/9/09 8:30	5.4	-0.1	275681	-26889	0
7/9/09 15:48	5.4	0.0	275681	-2521	0
8/4/09 23:45	5.4	0.0	275681	0	4201
8/5/09 23:45	5.3	0.0	275681	-4854	0
8/6/09 23:45	5.3	0.0	275681	-2735	0
8/7/09 23:45	5.3	0.0	275681	-2284	0
8/8/09 23:45	5.3	0.0	275681	-1169	0
8/9/09 23:45	5.3	0.0	275681	-356	0
8/10/09 23:45	5.2	0.0	275681	-1813	0
8/11/09 23:45	5.2	0.0	275681	-1640	0
8/12/09 23:45	5.2	0.0	275681	-1519	0
8/13/09 23:45	5.2	0.0	275681	-2167	0
8/14/09 23:45	5.2	0.0	275681	-1710	0
8/15/09 23:45	5.1	0.0	275681	-1580	0
8/16/09 23:45	5.1	0.0	275681	-2072	0
8/17/09 23:45	5.1	0.0	275681	-1813	0
8/20/09 23:45	5.1	0.0	275681	-1862	0
9/18/09 23:45	5.3	0.1	275681	0	16995
9/19/09 23:45	6.1	0.3	275681	0	69317
9/20/09 23:45	7.3	0.4	275681	0	103389
9/21/09 23:45	9.0	0.5	275681	0	142916
9/22/09 23:45	10.6	0.5	275681	0	133856
9/23/09 23:45	12.1	0.4	275681	0	123047
9/24/09 23:45	13.4	0.4	275681	0	113727
9/25/09 23:45	14.7	0.4	275681	0	106594
9/26/09 23:45	15.8	0.3	275681	0	91655
9/27/09 23:45	16.6	0.2	275681	0	66322
9/28/09 23:45	17.0	0.1	275681	0	35389
9/29/09 23:45	17.1	0.0	275681	0	10502
9/30/09 23:45	17.0	0.0	275681	-10396	0
10/1/09 23:45	16.7	-0.1	275681	-26512	0

TABLE C-2: 2009 INFLOW/OUTFLOW CALCULATIONS
Olin McIntosh Operable Unit 2, McIntosh, Alabama

Date	Basin Elevation (ft NAVD88)	Elevation Change from Previous Data Point (m)	Surface Area (m^2)	Incremental Outflow Volume (m^3)	Incremental Inflow Volume (m^3)
10/2/09 23:45	16.1	-0.2	275681	-51376	0
10/3/09 23:45	14.9	-0.4	275681	-102998	0
10/4/09 23:45	13.3	-0.5	275681	-130066	0
10/5/09 23:45	11.8	-0.5	275681	-124727	0
10/6/09 23:45	11.1	-0.2	275681	-59046	0
10/7/09 23:45	10.8	-0.1	275681	-25501	0
10/8/09 23:45	10.6	-0.1	275681	-18918	0
10/9/09 23:45	10.6	0.0	275681	-2155	0
10/10/09 23:45	11.1	0.2	275681	0	42864
10/11/09 23:45	11.4	0.1	275681	0	29147
10/12/09 23:45	11.4	0.0	275681	0	1396
10/13/09 23:45	11.3	0.0	275681	-11980	0
10/14/09 23:45	11.2	0.0	275681	-4714	0
10/15/09 23:45	12.0	0.2	275681	0	64536
10/16/09 23:45	13.2	0.4	275681	0	103626
10/17/09 23:45	14.4	0.3	275681	0	96259
10/18/09 23:45	15.5	0.3	275681	0	91166
10/19/09 23:45	16.4	0.3	275681	0	79956
10/20/09 23:45	17.2	0.2	275681	0	61057
10/21/09 23:45	17.6	0.1	275681	0	38667
10/22/09 23:45	17.8	0.1	275681	0	15288
10/23/09 23:45	17.7	0.0	275681	-10223	0
10/24/09 23:45	17.2	-0.1	275681	-38094	0
10/25/09 23:45	16.4	-0.3	275681	-72378	0
10/26/09 23:45	15.2	-0.3	275681	-93697	0
10/27/09 23:45	14.0	-0.4	275681	-105487	0
10/28/09 23:45	12.6	-0.4	275681	-119416	0
10/29/09 23:45	11.5	-0.3	275681	-90460	0
10/30/09 23:45	11.0	-0.1	275681	-40832	0
11/2/09 23:45	10.4	-0.2	275681	-49457	0
11/3/09 23:45	10.5	0.0	275681	0	5522
11/4/09 23:45	11.2	0.2	275681	0	56753
11/5/09 23:45	11.5	0.1	275681	0	29191
11/6/09 23:45	11.4	0.0	275681	-5503	0
11/7/09 23:45	11.3	-0.1	275681	-14968	0
11/8/09 23:45	10.9	-0.1	275681	-27852	0
11/9/09 23:45	10.7	-0.1	275681	-22203	0
11/10/09 23:45	10.4	-0.1	275681	-19840	0
11/11/09 23:45	10.1	-0.1	275681	-29735	0
11/12/09 23:45	11.1	0.3	275681	0	87574
11/13/09 23:45	12.9	0.5	275681	0	150190
11/14/09 23:45	14.3	0.4	275681	0	118617
11/15/09 23:45	15.5	0.4	275681	0	101987

TABLE C-2: 2009 INFLOW/OUTFLOW CALCULATIONS
Olin McIntosh Operable Unit 2, McIntosh, Alabama

Date	Basin Elevation (ft NAVD88)	Elevation Change from Previous Data Point (m)	Surface Area (m^2)	Incremental Outflow Volume (m^3)	Incremental Inflow Volume (m^3)
11/16/09 23:45	16.3	0.2	275681	0	67557
11/17/09 23:45	16.5	0.0	275681	0	11108
11/18/09 23:45	15.9	-0.2	275681	-44678	0
11/19/09 23:45	15.3	-0.2	275681	-55805	0
11/20/09 23:45	14.6	-0.2	275681	-56127	0
11/21/09 23:45	13.8	-0.2	275681	-63577	0
11/22/09 23:45	13.0	-0.3	275681	-69503	0
11/23/09 23:45	12.0	-0.3	275681	-81932	0
11/24/09 23:45	11.3	-0.2	275681	-64569	0
11/25/09 23:45	10.9	-0.1	275681	-33140	0
11/26/09 23:45	10.6	-0.1	275681	-21477	0
11/27/09 23:45	10.5	-0.1	275681	-14646	0
11/28/09 23:45	10.4	0.0	275681	-7607	0
11/29/09 23:45	10.3	0.0	275681	-7968	0
11/30/09 23:45	9.8	-0.1	275681	-36982	0
12/1/09 23:45	9.3	-0.2	275681	-41854	0
12/2/09 23:45	9.0	-0.1	275681	-30698	0
12/3/09 8:00	9.0	0.0	275681	0	2998
12/4/09 8:35	10.4	0.4	275681	0	117639
12/5/09 10:00	11.2	0.2	275681	0	67222
12/6/09 10:35	11.3	0.0	275681	0	8403
12/7/09 9:00	11.3	0.0	275681	0	0
12/8/09 9:30	11.1	-0.1	275681	-16806	0
12/9/09 10:30	11.0	0.0	275681	-8403	0
12/10/09 8:30	11.5	0.2	275681	0	42014
12/11/09 9:00	12.7	0.4	275681	0	100833
12/12/09 16:15	14.2	0.5	275681	0	126041
12/13/09 14:30	15.7	0.5	275681	0	126041
12/14/09 7:30	16.7	0.3	275681	0	84028
12/14/09 7:30	*16.7*	0.0	275681	0	0
12/15/09 0:00	*17.4*	0.2	275681	0	58819
12/16/09 0:00	*17.3*	0.0	275681	-8403	0
12/17/09 0:00	*17.2*	0.0	275681	-8403	0
12/18/09 0:00	*17.1*	0.0	275681	-8403	0
12/19/09 0:00	*17.0*	0.0	275681	-8403	0
12/20/09 0:00	*16.9*	0.0	275681	-8403	0
12/21/09 0:00	*16.7*	-0.1	275681	-16806	0
12/22/09 0:00	*16.5*	-0.1	275681	-16806	0
12/23/09 0:00	*16.1*	-0.1	275681	-33611	0
12/24/09 0:00	*15.6*	-0.2	275681	-42014	0
12/25/09 0:00	*15.0*	-0.2	275681	-50417	0
12/26/09 0:00	*16.0*	0.3	275681	0	84028

TABLE C-2: 2009 INFLOW/OUTFLOW CALCULATIONS
Olin McIntosh Operable Unit 2, McIntosh, Alabama

Date	Basin Elevation (ft NAVD88)	Elevation Change from Previous Data Point (m)	Surface Area (m^2)	Incremental Outflow Volume (m^3)	Incremental Inflow Volume (m^3)
12/27/09 0:00	*15.1*	-0.3	275681	-75625	0
12/28/09 0:00	*14.7*	-0.1	275681	-33611	0
12/29/09 0:00	*14.0*	-0.2	275681	-58819	0
12/30/09 0:00	*14.9*	0.3	275681	0	75625
12/31/09 0:00	*15.9*	0.3	275681	0	84028
2008 TOTALS				-6476428	7115038
			Inflow/Outflow = (Outflow sum + |Inflow Sum|) ÷ 2 =		**6,795,733**

Prepared/Date: KPW 05/25/11
Checked/Date: NTG 05/25/11

Note: *Dates and elevations in italics indicate estimated elevations.*

Figure C-1: 2008 Basin Water Elevations Used to Calculate Inflow/Outflow

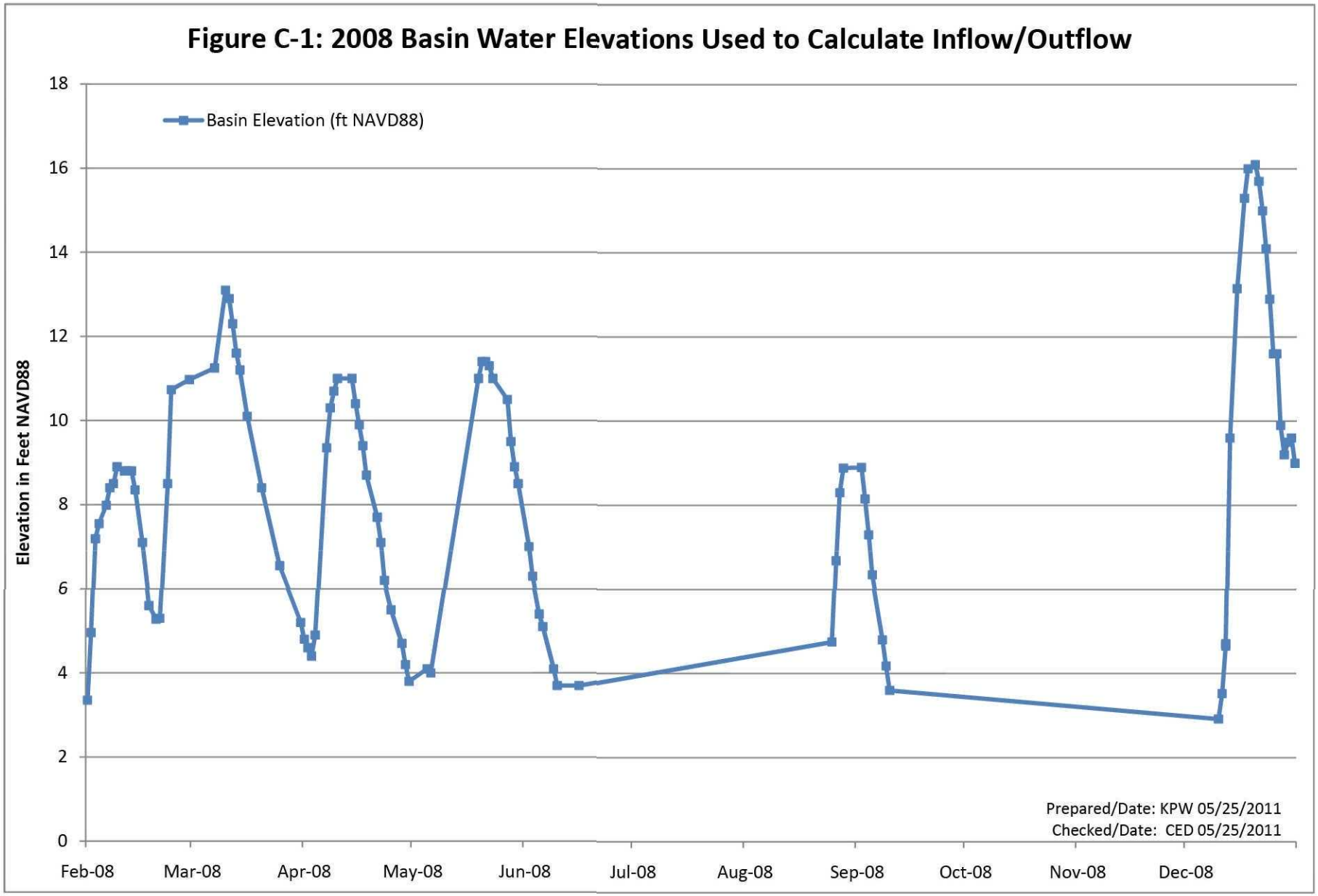
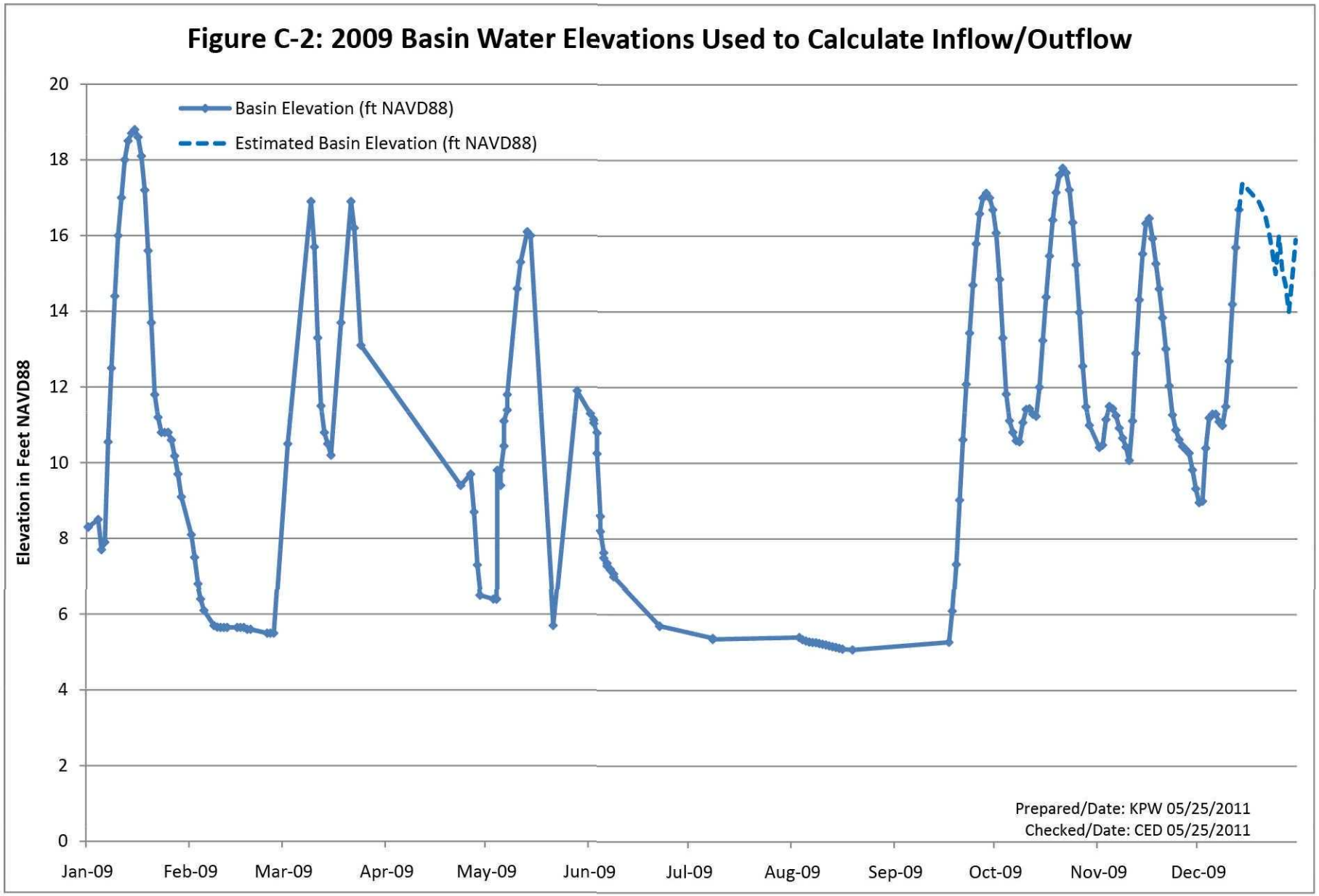


Figure C-2: 2009 Basin Water Elevations Used to Calculate Inflow/Outflow



Legend

- Interpolated 6 Foot Contour Within the Berm
- Interpolated 3 Foot Contour Within the Basin
- 2006 Bathymetric Survey (Elevations in NAVD 88)

ROUND POND

BASIN

INLET CHANNEL

TOMBIGBEE RIVER

0 200 400 600 800 Feet

Source: USDA/FSA - Aerial Photography Field Office - 2009

Olin McIntosh OU 2

Water Elevations Used in SERAFM Scenarios

Prepared by/Date: THP - 3/21/11	MACTEC	Figure Number: C-3
Checked by: CED - 3/21/11		
Project Number: 6107110036		

Path: G:\Projects_GIS\Projects2007\olin_mcintosh\Report mxds\RI Addendum 3_16_11\report mxds\WaterElev_Serafm_Scenarios.mxd

APPENDIX D-1

Terrestrial Data Pairings and Regression Plots – Invertebrate Tissue and Surface Soil

TABLE D-1

Data Pairing for Mercury in Terrestrial Invertebrates
OLIN McINTOSH OU-2

Sample Type	Number of Soil Samples	Parameter	Soil Sample IDs	Soil Concentration (mg/kg)	Average Soil Concentration (mg/kg)	Hg (Total) Tissue Concentration (mg/kg)	Methylmercury Tissue Concentration (mg/kg) (a)	Insect Sample IDs
Flying Insect	1	Hg/MeHg	OU2B-FPSS6-10	0.16	0.16	0.32	0.15	OU2B-INS1B-10
Crawling Insect	2	Hg/MeHg	OU2B-FPSS4-10 OU2B-FPSSDUP01-10 OU2B-FPSS3-10	0.20 0.27 1.6	0.92 (b)	0.37	0.17	OU2B-INS2C-10
Flying Insect	3	Hg/MeHg	OU2B-FPSB3-10-0-1 OU2B-FPSBDUP02-10 OU2B-FPSS7-10 OU2B-FPSS8-10	0.20 0.044 1.1 0.15	0.46 (b)	0.31	0.15	OU2B-INS3B-10
Flying Insect	1	Hg/MeHg	OU2B-FPSS11-10	1.0	1.0	0.26	0.12	OU2B-INS4B-10
Crawling Insect	1	Hg/MeHg	OU2B-FPSS11-10	1.0	1.0	0.0075	0.0035	OU2B-INS4C-10
Flying Insect	1	Hg/MeHg	OU2B-FPSB5-10-0-1 OU2B-FPSBDUP03-10	2.4 2.5	2.45 (b)	0.14	0.066	OU2B-INS5B-10
Crawling Insect	1	Hg/MeHg	OU2B-FPSB5-10-0-1 OU2B-FPSBDUP03-10	2.4 2.5	2.45 (b)	0.067	0.031	OU2B-INS5C-10
Spider	2	Hg/MeHg	OU2B-FPSS13-10 OU2B-FPSS14-10 OU2B-FPSSDUP02-10	1.6 1.7 1.8	1.68 (b)	0.15	0.071	OU2B-INS6A-10
Flying Insect	2	Hg/MeHg	OU2B-FPSS13-10 OU2B-FPSS14-10 OU2B-FPSSDUP02-10	1.6 1.7 1.8	1.68 (b)	0.71	0.33	OU2B-INS6B-10
Crawling Insect	2	Hg/MeHg	OU2B-FPSS13-10 OU2B-FPSS14-10 OU2B-FPSSDUP02-10	1.6 1.7 1.8	1.68 (b)	0.026	0.012	OU2B-INS6C-10
Spider (Northeast)	6	Hg/MeHg	OU2B-FPSS6-10 OU2B-FPSS4-10 OU2B-FPSSDUP01-10 OU2B-FPSB3-10-0-1 OU2B-FPSBDUP02-10 OU2B-FPSS8-10 OU2B-FPSS7-10 OU2B-FPSS3-10	0.16 0.20 0.27 0.20 0.044 0.15 1.1 1.6	0.56 (b)	0.17	0.080	OU2B-INSNEA-10

TABLE D-1

Data Pairing for Mercury in Terrestrial Invertebrates
OLIN McINTOSH OU-2

Sample Type	Number of Soil Samples	Parameter	Soil Sample IDs	Soil Concentration (mg/kg)	Average Soil Concentration (mg/kg)	Hg (Total) Tissue Concentration (mg/kg)	Methylmercury Tissue Concentration (mg/kg) (a)	Insect Sample IDs
Crawling Insect (Northeast)	6	Hg/MeHg	OU2B-FPSS6-10 OU2B-FPSS4-10 OU2B-FPSSDUP01-10 OU2B-FPSB3-10-0-1 OU2B-FPSBDUP02-10 OU2B-FPSS8-10 OU2B-FPSS7-10 OU2B-FPSS3-10	0.16 0.20 0.27 0.20 0.044 0.15 1.1 1.6	0.56 (b)	0.075	0.035	OU2B-INSNEC-10
Spider (Southeast)	3	Hg/MeHg	OU2B-FPSS11-10 OU2B-FPSB5-10-0-1 OU2B-FPSBDUP03-10 OU2B-FPSS12-10	1.0 2.4 2.5 0.42	1.29 (b)	0.13	0.061	OU2B-INSSEA-10
Insects - composite (c) (1994- Southwest)	3	Hg/MeHg	OSG0701-0694 OSG0701FD-0694 OSG0702-0694 OSG0703-0694	4.0 5.1 2.7 4.1	3.78 (b)	0.14	0.066	OIN0303

Notes:
(a) MeHg assumed to be 47% of Total Mercury. MeHg in Tissue not analyzed directly.
(b) Concentration includes an average of a parent sample and a duplicate sample.
(c) Terrestrial insects from 1994 include crawling, climbing, and flying insects composited together. This sample will be combined with the complete dataset for the purposes of BAF analysis; however, the sample will not be included when considering individual types of insects.

PREPARED BY/DATE: MKB 1/23/12
CHECKED BY/DATE: NSR 1/23/12

A = Spiders
B = Flying Insects
C = Crawling Insects

TABLE D-2

Data Pairing for DDT Isomers in Terrestrial Invertebrates*

OLIN McINTOSH OU-2

Sample Type	Number of Soil Samples	Parameter	Soil Sample IDs	Individual Soil Concentrations (ug/kg)	Representative Soil Concentration (ug/kg) [a]	Representative Soil Concentration (mg/kg)	TOC (mg/kg)	FOC	Norm. Soil Concentration (mg/kg)	Tissue Concentration (ug/kg)	Tissue Concentration (mg/kg)	Fraction Lipids	Norm. Tissue Concentration (mg/kg)	Insect Sample IDs
Flying Insect	1	2,4'-DDD	OU2B-FPSS6-10	NA	9.6	0.0096	59600	0.0596	0.16	5.4	0.0054	0.032	0.17	OU2B-INS1B-10
		2,4'-DDE	OU2B-FPSS6-10	NA	8.3	0.008	59600	0.0596	0.14	16.8	0.017	0.032	0.53	OU2B-INS1B-10
		2,4'-DDT	OU2B-FPSS6-10	NA	11.5	0.012	59600	0.0596	0.19	0.7	0.00068	0.032	0.02	OU2B-INS1B-10
		4,4'-DDD	OU2B-FPSS6-10	NA	29.7	0.030	59600	0.0596	0.50	14	0.014	0.032	0.44	OU2B-INS1B-10
		4,4'-DDE	OU2B-FPSS6-10	NA	18.6	0.019	59600	0.0596	0.31	606	0.61	0.032	18.94	OU2B-INS1B-10
		4,4'-DDT	OU2B-FPSS6-10	NA	138	0.14	59600	0.0596	2.32	16.6	0.017	0.032	0.52	OU2B-INS1B-10
		DDTR [b]	**OU2B-FPSS6-10**			**0.22**			**3.62**		**0.66**		**20.6**	**OU2B-INS1B-10**
Crawling Insect	2	2,4'-DDD	OU2B-FPSS4-10	6.2	7.65	0.0077	50500	0.0505	0.15	5.2	0.005	0.033	0.16	OU2B-INS2C-10
			OU2B-FPSSDUP01-10	9.1										
		2,4'-DDE	OU2B-FPSS4-10	4.6	5.85	0.0059	50500	0.0505	0.12	13.8	0.014	0.033	0.42	OU2B-INS2C-10
			OU2B-FPSSDUP01-10	7.1										
		2,4'-DDT	OU2B-FPSS4-10	*0.65*	*0.675*	*0.00068*	50500	0.0505	0.013	*1.25*	*0.001*	0.033	0.038	OU2B-INS2C-10
			OU2B-FPSSDUP01-10	*0.70*										
		4,4'-DDD	OU2B-FPSS4-10	19.6	20.4	0.020	50500	0.0505	0.40	11.3	0.011	0.033	0.34	OU2B-INS2C-10
			OU2B-FPSSDUP01-10	21.1										
		4,4'-DDE	OU2B-FPSS4-10	10.3	11.3	0.011	50500	0.0505	0.22	318	0.318	0.033	9.64	OU2B-INS2C-10
			OU2B-FPSSDUP01-10	12.2										
		4,4'-DDT	OU2B-FPSS4-10	52.6	31.1	0.031	50500	0.0505	0.62	4.0	0.0040	0.033	0.12	OU2B-INS2C-10
			OU2B-FPSSDUP01-10	9.6										
		DDTR [b]	**OU2B-FPSS4-10**			**0.077**			**1.52**					
		2,4'-DDD	OU2B-FPSS3-10	NA	71.6	0.0716	298000	0.298	0.24					
		2,4'-DDE	OU2B-FPSS3-10	NA	54.1	0.0541	298000	0.298	0.18					
		2,4'-DDT	OU2B-FPSS3-10	NA	*3.3*	*0.0033*	298000	0.298	0.011					
		4,4'-DDD	OU2B-FPSS3-10	NA	104	0.104	298000	0.298	0.35					
		4,4'-DDE	OU2B-FPSS3-10	NA	98.9	0.0989	298000	0.298	0.33					
		4,4'-DDT	OU2B-FPSS3-10	NA	*3.3*	0.0033	298000	0.298	0.01					
		DDTR [b]	**OU2B-FPSS3-10**			**0.335**			**1.12**					
		DDTR [b]				**0.206**			**1.32**		**0.35**		**10.7**	**OU2B-INS2C-10**
Flying Insect	3	2,4'-DDD	OU2B-FPSB3-10-0-1	4.0	3.75	0.0038	41300	0.0413	0.09	6.0	0.006	0.040	0.15	OU2B-INS3B-10
			OU2B-FPSBDUP02-10	3.5										
		2,4'-DDE	OU2B-FPSB3-10-0-1	4.2	4.05	0.0041	41300	0.0413	0.10	29.2	0.029	0.040	0.73	OU2B-INS3B-10
			OU2B-FPSBDUP02-10	3.9										
		2,4'-DDT	OU2B-FPSB3-10-0-1	1.7	3.5	0.0035	41300	0.0413	0.08	0.72	0.001	0.040	0.02	OU2B-INS3B-10
			OU2B-FPSBDUP02-10	5.3										
		4,4'-DDD	OU2B-FPSB3-10-0-1	10.2	8.6	0.009	41300	0.0413	0.21	10	0.010	0.040	0.25	OU2B-INS3B-10
			OU2B-FPSBDUP02-10	7.0										
		4,4'-DDE	OU2B-FPSB3-10-0-1	16.6	13.4	0.013	41300	0.0413	0.32	288	0.288	0.040	7.20	OU2B-INS3B-10
			OU2B-FPSBDUP02-10	10.1										
		4,4'-DDT	OU2B-FPSB3-10-0-1	11.8	18.1	0.018	41300	0.0413	0.44	3.3	0.0033	0.040	0.08	OU2B-INS3B-10
			OU2B-FPSBDUP02-10	24.3										
		DDTR [b]	**OU2B-FPSB3-10**			**0.051**			**1.24**					
		2,4'-DDD	OU2B-FPSS8-10	NA	36.3	0.0363	56400	0.0564	0.64					
		2,4'-DDE	OU2B-FPSS8-10	NA	31.1	0.0311	56400	0.0564	0.55					
		2,4'-DDT	OU2B-FPSS8-10	NA	5.7	0.0057	56400	0.0564	0.10					
		4,4'-DDD	OU2B-FPSS8-10	NA	83.5	0.0835	56400	0.0564	1.48					
		4,4'-DDE	OU2B-FPSS8-10	NA	74	0.074	56400	0.0564	1.31					
		4,4'-DDT	OU2B-FPSS8-10	NA	64.1	0.0641	56400	0.0564	1.14					
		DDTR [b]	**OU2B-FPSS8-10**			**0.295**			**5.23**					
		2,4'-DDD	OU2B-FPSS7-10	NA	5.2	0.0052	42900	0.0429	0.12					
		2,4'-DDE	OU2B-FPSS7-10	NA	7.0	0.0070	42900	0.0429	0.16					
		2,4'-DDT	OU2B-FPSS7-10	NA	4.2	0.0042	42900	0.0429	0.10					
		4,4'-DDD	OU2B-FPSS7-10	NA	14.3	0.0143	42900	0.0429	0.33					
		4,4'-DDE	OU2B-FPSS7-10	NA	19	0.019	42900	0.0429	0.44					
		4,4'-DDT	OU2B-FPSS7-10	NA	5.6	0.0056	42900	0.0429	0.13					
		DDTR [b]	**OU2B-FPSS7-10**			**0.055**			**1.29**					
		DDTR [b]				**0.134**			**2.59**		**0.34**		**8.4**	**OU2B-INS3B-10**

TABLE D-2

Data Pairing for DDT Isomers in Terrestrial Invertebrates*

OLIN McINTOSH OU-2

Sample Type	Number of Soil Samples	Parameter	Soil Sample IDs	Individual Soil Concentrations (ug/kg)	Representative Soil Concentration (ug/kg) [a]	Representative Soil Concentration (mg/kg)	TOC (mg/kg)	FOC	Norm. Soil Concentration (mg/kg)	Tissue Concentration (ug/kg)	Tissue Concentration (mg/kg)	Fraction Lipids	Norm. Tissue Concentration (mg/kg)	Insect Sample IDs
Flying Insect	1	2,4'-DDD	OU2B-FPSS11-10	NA	4.9	0.0049	31100	0.0311	0.16	4.4	0.0044	0.041	0.11	OU2B-INS4B-10
		2,4'-DDE	OU2B-FPSS11-10	NA	7.7	0.0077	31100	0.0311	0.25	22.5	0.023	0.041	0.55	OU2B-INS4B-10
		2,4'-DDT	OU2B-FPSS11-10	NA	*0.44*	*0.0004*	31100	0.0311	0.014	0.70	0.00070	0.041	0.02	OU2B-INS4B-10
		4,4'-DDD	OU2B-FPSS11-10	NA	7.8	0.0078	31100	0.0311	0.25	12.1	0.012	0.041	0.30	OU2B-INS4B-10
		4,4'-DDE	OU2B-FPSS11-10	NA	14.6	0.0146	31100	0.0311	0.47	233	0.23	0.041	5.68	OU2B-INS4B-10
		4,4'-DDT	OU2B-FPSS11-10	NA	*0.44*	*0.0004*	31100	0.0311	0.014	9.4	0.0094	0.041	0.23	OU2B-INS4B-10
		DDTR [b]				**0.036**			**1.15**		**0.28**		**6.9**	**OU2B-INS4B-10**
Crawling Insect	1	2,4'-DDD	OU2B-FPSS11-10	NA	4.9	0.0049	31100	0.0311	0.16	*2.5*	*0.0025*	0.028	0.089	OU2B-INS4C-10
		2,4'-DDE	OU2B-FPSS11-10	NA	7.7	0.0077	31100	0.0311	0.25	4.1	0.0041	0.028	0.15	OU2B-INS4C-10
		2,4'-DDT	OU2B-FPSS11-10	NA	*0.44*	*0.0004*	31100	0.0311	0.014	*2.50*	*0.0025*	0.028	0.089	OU2B-INS4C-10
		4,4'-DDD	OU2B-FPSS11-10	NA	7.8	0.0078	31100	0.0311	0.25	*4.95*	*0.0050*	0.028	0.18	OU2B-INS4C-10
		4,4'-DDE	OU2B-FPSS11-10	NA	14.6	0.0146	31100	0.0311	0.47	*4.95*	*0.0050*	0.028	0.18	OU2B-INS4C-10
		4,4'-DDT	OU2B-FPSS11-10	NA	*0.44*	*0.0004*	31100	0.0311	0.014	*4.95*	*0.0050*	0.028	0.18	OU2B-INS4C-10
		DDTR [b]				**0.036**			**1.15**		**0.0240**		**0.86**	**OU2B-INS4C-10**
Flying Insect	1	2,4'-DDD	OU2B-FPSS12-10	NA	0.68	0.00068	15900	0.0159	0.043	4.5	0.0045	0.04	0.113	OU2B-INS5B-10
		2,4'-DDE	OU2B-FPSS12-10	NA	0.85	0.00085	15900	0.0159	0.053	22.6	0.0226	0.04	0.57	OU2B-INS5B-10
		2,4'-DDT	OU2B-FPSS12-10	NA	*0.38*	*0.00038*	15900	0.0159	0.024	0.91	0.0009	0.04	0.023	OU2B-INS5B-10
		4,4'-DDD	OU2B-FPSS12-10	NA	1.3	0.0013	15900	0.0159	0.082	3.3	0.0033	0.04	0.08	OU2B-INS5B-10
		4,4'-DDE	OU2B-FPSS12-10	NA	0.95	0.00095	15900	0.0159	0.060	86.6	0.0866	0.04	2.17	OU2B-INS5B-10
		4,4'-DDT	OU2B-FPSS12-10	NA	1.8	0.0018	15900	0.0159	0.113	2.4	0.0024	0.04	0.06	OU2B-INS5B-10
		***DDTR* [b]**				***0.0060***			**0.37**		**0.12**		**3.01**	**OU2B-INS5B-10**
Crawling Insect	1	2,4'-DDD	OU2B-FPSS12-10	NA	0.68	0.00068	15900	0.0159	0.043	*1.9*	*0.0019*	0.033	0.058	OU2B-INS5C-10
		2,4'-DDE	OU2B-FPSS12-10	NA	0.85	0.00085	15900	0.0159	0.053	*1.9*	*0.0019*	0.033	0.058	OU2B-INS5C-10
		2,4'-DDT	OU2B-FPSS12-10	NA	*0.38*	*0.00038*	15900	0.0159	0.024	*1.9*	*0.0019*	0.033	0.058	OU2B-INS5C-10
		4,4'-DDD	OU2B-FPSS12-10	NA	1.3	0.0013	15900	0.0159	0.082	2.2	0.0022	0.033	0.067	OU2B-INS5C-10
		4,4'-DDE	OU2B-FPSS12-10	NA	0.95	0.00095	15900	0.0159	0.060	5.3	0.0053	0.033	0.16	OU2B-INS5C-10
		4,4'-DDT	OU2B-FPSS12-10	NA	1.8	0.0018	15900	0.0159	0.113	2.0	0.0020	0.033	0.06	OU2B-INS5C-10
		DDTR [b]				**0.0060**			**0.37**		**0.02**		**0.46**	**OU2B-INS5C-10**
Spider (Northeast)	6	2,4'-DDD	OU2B-FPSS6-10	NA	9.6	0.010	59600	0.0596	0.16	1.9	0.0019	0.035	0.054	OU2B-INSNEA-10
		2,4'-DDE	OU2B-FPSS6-10	NA	8.3	0.0083	59600	0.0596	0.14	6.4	0.0064	0.035	0.18	OU2B-INSNEA-10
		2,4'-DDT	OU2B-FPSS6-10	NA	11.5	0.0115	59600	0.0596	0.19	1.0	0.0010	0.035	0.029	OU2B-INSNEA-10
		4,4'-DDD	OU2B-FPSS6-10	NA	29.7	0.0297	59600	0.0596	0.50	21	0.021	0.035	0.59	OU2B-INSNEA-10
		4,4'-DDE	OU2B-FPSS6-10	NA	18.6	0.0186	59600	0.0596	0.31	301	0.30	0.035	8.6	OU2B-INSNEA-10
		4,4'-DDT	OU2B-FPSS6-10	NA	138	0.1380	59600	0.0596	2.32	4.0	0.004	0.035	0.11	OU2B-INSNEA-10
		DDTR [b]	**OU2B-FPSS6-10**			**0.22**			**3.62**					
		2,4'-DDD	OU2B-FPSB3-10-0-1	4.0	3.75	0.0038	41300	0.0413	0.09					
			OU2B-FPSBDUP02-10	3.5										
		2,4'-DDE	OU2B-FPSB3-10-0-1	4.2	4.05	0.0041	41300	0.0413	0.10					
			OU2B-FPSBDUP02-10	3.9										
		2,4'-DDT	OU2B-FPSB3-10-0-1	1.7	3.5	0.0035	41300	0.0413	0.08					
			OU2B-FPSBDUP02-10	5.3										
		4,4'-DDD	OU2B-FPSB3-10-0-1	10.2	8.6	0.009	41300	0.0413	0.21					
			OU2B-FPSBDUP02-10	7.0										
		4,4'-DDE	OU2B-FPSB3-10-0-1	16.6	13.4	0.013	41300	0.0413	0.32					
			OU2B-FPSBDUP02-10	10.1										
		4,4'-DDT	OU2B-FPSB3-10-0-1	11.8	18.1	0.018	41300	0.0413	0.44					
			OU2B-FPSBDUP02-10	24.3										
		DDTR [b]	**OU2B-FPSB3-10-0-1**			**0.051**			**1.24**					
		2,4'-DDD	OU2B-FPSS4-10	6.2	7.65	0.0077	50500	0.0505	0.15					
			OU2B-FPSSDUP01-10	9.1										
		2,4'-DDE	OU2B-FPSS4-10	4.6	5.85	0.0059	50500	0.0505	0.12					
			OU2B-FPSSDUP01-10	7.1										
		2,4'-DDT	OU2B-FPSS4-10	*0.65*	*0.675*	*0.00068*	50500	0.0505	0.013					
			OU2B-FPSSDUP01-10	*0.70*										
		4,4'-DDD	OU2B-FPSS4-10	19.6	20.4	0.020	50500	0.0505	0.40					
			OU2B-FPSSDUP01-10	21.1										
		4,4'-DDE	OU2B-FPSS4-10	10.3	11.3	0.011	50500	0.0505	0.22					
			OU2B-FPSSDUP01-10	12.2										
		4,4'-DDT	OU2B-FPSS4-10	52.6	31.1	0.031	50500	0.0505	0.62					
			OU2B-FPSSDUP01-10	9.6										
		DDTR [b]	**OU2B-FPSS4-10**			**0.077**			**1.52**					

TABLE D-2

Data Pairing for DDT Isomers in Terrestrial Invertebrates*

OLIN McINTOSH OU-2

Sample Type	Number of Soil Samples	Parameter	Soil Sample IDs	Individual Soil Concentrations (ug/kg)	Representative Soil Concentration (ug/kg) [a]	Representative Soil Concentration (mg/kg)	TOC (mg/kg)	FOC	Norm. Soil Concentration (mg/kg)	Tissue Concentration (ug/kg)	Tissue Concentration (mg/kg)	Fraction Lipids	Norm. Tissue Concentration (mg/kg)	Insect Sample IDs
Spider (Northeast) (Cont.)	6	2,4'-DDD	OU2B-FPSS8-10	NA	36.3	0.0363	56400	0.0564	0.64					
		2,4'-DDE	OU2B-FPSS8-10	NA	31.1	0.0311	56400	0.0564	0.55					
		2,4'-DDT	OU2B-FPSS8-10	NA	5.7	0.0057	56400	0.0564	0.10					
		4,4'-DDD	OU2B-FPSS8-10	NA	83.5	0.0835	56400	0.0564	1.48					
		4,4'-DDE	OU2B-FPSS8-10	NA	74	0.074	56400	0.0564	1.31					
		4,4'-DDT	OU2B-FPSS8-10	NA	64.1	0.0641	56400	0.0564	1.14					
		DDTR [b]	**OU2B-FPSS8-10**			**0.295**			**5.23**					
		2,4'-DDD	OU2B-FPSS7-10	NA	5.2	0.0052	42900	0.0429	0.12					
		2,4'-DDE	OU2B-FPSS7-10	NA	7.0	0.0070	42900	0.0429	0.16					
		2,4'-DDT	OU2B-FPSS7-10	NA	4.2	0.0042	42900	0.0429	0.10					
		4,4'-DDD	OU2B-FPSS7-10	NA	14.3	0.0143	42900	0.0429	0.33					
		4,4'-DDE	OU2B-FPSS7-10	NA	19	0.019	42900	0.0429	0.44					
		4,4'-DDT	OU2B-FPSS7-10	NA	5.6	0.0056	42900	0.0429	0.13					
		DDTR [b]	**OU2B-FPSS7-10**			**0.055**			**1.29**					
		2,4'-DDD	OU2B-FPSS3-10	NA	71.6	0.0716	298000	0.298	0.24					
		2,4'-DDE	OU2B-FPSS3-10	NA	54.1	0.0541	298000	0.298	0.18					
		2,4'-DDT	OU2B-FPSS3-10	NA	*3.3*	*0.0033*	298000	0.298	0.011					
		4,4'-DDD	OU2B-FPSS3-10	NA	104	0.104	298000	0.298	0.35					
		4,4'-DDE	OU2B-FPSS3-10	NA	98.9	0.0989	298000	0.298	0.33					
		4,4'-DDT	OU2B-FPSS3-10	NA	*3.3*	0.0033	298000	0.298	0.011					
		DDTR [b]	**OU2B-FPSS3-10**			**0.335**			**1.12**					
AVEREAGE DDTR (Northeast) [c]						**0.172**			**2.34**		**0.33**		**9.57**	**OU2B-INSNEA-10**
Crawling Insect (Northeast)	6	2,4'-DDD	OU2B-FPSS6-10	NA	9.6	0.010	59600	0.0596	0.16	3.5	0.0035	0.044	0.080	OU2B-INSNEC-10
		2,4'-DDE	OU2B-FPSS6-10	NA	8.3	0.008	59600	0.0596	0.14	5.4	0.0054	0.044	0.12	OU2B-INSNEC-10
		2,4'-DDT	OU2B-FPSS6-10	NA	11.5	0.012	59600	0.0596	0.19	*2.3*	*0.0023*	0.044	0.052	OU2B-INSNEC-10
		4,4'-DDD	OU2B-FPSS6-10	NA	29.7	0.030	59600	0.0596	0.50	5.2	0.0052	0.044	0.12	OU2B-INSNEC-10
		4,4'-DDE	OU2B-FPSS6-10	NA	18.6	0.019	59600	0.0596	0.31	30.7	0.031	0.044	0.70	OU2B-INSNEC-10
		4,4'-DDT	OU2B-FPSS6-10	NA	138	0.138	59600	0.0596	2.32	1.5	0.0015	0.044	0.034	OU2B-INSNEC-10
		DDTR	**OU2B-FPSS6-10**			**0.22**			**3.62**					
		2,4'-DDD	OU2B-FPSB3-10-0-1	4.0	3.75	0.0038	41300	0.0413	0.09					
			OU2B-FPSBDUP02-10	3.5										
		2,4'-DDE	OU2B-FPSB3-10-0-1	4.2	4.05	0.0041	41300	0.0413	0.10					
			OU2B-FPSBDUP02-10	3.9										
		2,4'-DDT	OU2B-FPSB3-10-0-1	1.7	3.5	0.0035	41300	0.0413	0.08					
			OU2B-FPSBDUP02-10	5.3										
		4,4'-DDD	OU2B-FPSB3-10-0-1	10.2	8.6	0.009	41300	0.0413	0.21					
			OU2B-FPSBDUP02-10	7.0										
		4,4'-DDE	OU2B-FPSB3-10-0-1	16.6	13.4	0.013	41300	0.0413	0.32					
			OU2B-FPSBDUP02-10	10.1										
		4,4'-DDT	OU2B-FPSB3-10-0-1	11.8	18.1	0.018	41300	0.0413	0.44					
			OU2B-FPSBDUP02-10	24.3										
		DDTR	**OU2B-FPSB3-10-0-1**			**0.051**			**1.24**					
		2,4'-DDD	OU2B-FPSS4-10	6.2	7.65	0.0077	50500	0.0505	0.15					
			OU2B-FPSSDUP01-10	9.1										
		2,4'-DDE	OU2B-FPSS4-10	4.6	5.85	0.0059	50500	0.0505	0.12					
			OU2B-FPSSDUP01-10	7.1										
		2,4'-DDT	OU2B-FPSS4-10	*0.65*	*0.675*	*0.00068*	50500	0.0505	0.013					
			OU2B-FPSSDUP01-10	*0.70*										
		4,4'-DDD	OU2B-FPSS4-10	19.6	20.4	0.020	50500	0.0505	0.40					
			OU2B-FPSSDUP01-10	21.1										
		4,4'-DDE	OU2B-FPSS4-10	10.3	11.3	0.011	50500	0.0505	0.22					
			OU2B-FPSSDUP01-10	12.2										
		4,4'-DDT	OU2B-FPSS4-10	52.6	31.1	0.031	50500	0.0505	0.62					
			OU2B-FPSSDUP01-10	9.6										
		DDTR	**OU2B-FPSS4-10**			**0.077**			**1.52**					
		2,4'-DDD	OU2B-FPSS8-10	NA	36.3	0.0363	56400	0.0564	0.64					
		2,4'-DDE	OU2B-FPSS8-10	NA	31.1	0.0311	56400	0.0564	0.55					
		2,4'-DDT	OU2B-FPSS8-10	NA	5.7	0.0057	56400	0.0564	0.10					
		4,4'-DDD	OU2B-FPSS8-10	NA	83.5	0.0835	56400	0.0564	1.48					
		4,4'-DDE	OU2B-FPSS8-10	NA	74	0.074	56400	0.0564	1.31					
		4,4'-DDT	OU2B-FPSS8-10	NA	64.1	0.0641	56400	0.0564	1.14					

TABLE D-2

Data Pairing for DDT Isomers in Terrestrial Invertebrates*

OLIN McINTOSH OU-2

Sample Type	Number of Soil Samples	Parameter	Soil Sample IDs	Individual Soil Concentrations (ug/kg)	Representative Soil Concentration (ug/kg) [a]	Representative Soil Concentration (mg/kg)	TOC (mg/kg)	FOC	Norm. Soil Concentration (mg/kg)	Tissue Concentration (ug/kg)	Tissue Concentration (mg/kg)	Fraction Lipids	Norm. Tissue Concentration (mg/kg)	Insect Sample IDs
Crawling Insect (Northeast) (Cont.)	6	**DDTR [b]**	**OU2B-FPSS8-10**			**0.295**			**5.23**					
		2,4'-DDD	OU2B-FPSS7-10	NA	5.2	0.0052	42900	0.0429	0.12					
		2,4'-DDE	OU2B-FPSS7-10	NA	7.0	0.0070	42900	0.0429	0.16					
		2,4'-DDT	OU2B-FPSS7-10	NA	4.2	0.0042	42900	0.0429	0.10					
		4,4'-DDD	OU2B-FPSS7-10	NA	14.3	0.0143	42900	0.0429	0.33					
		4,4'-DDE	OU2B-FPSS7-10	NA	19	0.019	42900	0.0429	0.44					
		4,4'-DDT	OU2B-FPSS7-10	NA	5.6	0.0056	42900	0.0429	0.13					
		DDTR [b]	**OU2B-FPSS7-10**			**0.055**			**1.29**					
		2,4'-DDD	OU2B-FPSS3-10	NA	71.6	0.0716	298000	0.298	0.24					
		2,4'-DDE	OU2B-FPSS3-10	NA	54.1	0.0541	298000	0.298	0.18					
		2,4'-DDT	OU2B-FPSS3-10	NA	*3.3*	*0.0033*	298000	0.298	0.011					
		4,4'-DDD	OU2B-FPSS3-10	NA	104	0.104	298000	0.298	0.35					
		4,4'-DDE	OU2B-FPSS3-10	NA	98.9	0.0989	298000	0.298	0.33					
		4,4'-DDT	OU2B-FPSS3-10	NA	*3.3*	0.0033	298000	0.298	0.011					
		DDTR [b]	**OU2B-FPSS3-10**			**0.335**			**1.12**					
AVEREAGE DDTR (Northeast) [c]						**0.172**			**2.34**		**0.049**		**1.10**	**OU2B-INSNEC-10**
Spider (Southeast)	1	2,4'-DDD	OU2B-FPSS11-10	NA	4.9	0.0049	31100	0.0311	0.16	1.3	0.0013	0.036	0.036	OU2B-INSSEA-10
		2,4'-DDE	OU2B-FPSS11-10	NA	7.7	0.0077	31100	0.0311	0.25	7.7	0.0077	0.036	0.21	OU2B-INSSEA-10
		2,4'-DDT	OU2B-FPSS11-10	NA	*0.44*	*0.0004*	31100	0.0311	0.014	*1.25*	*0.0013*	0.036	0.035	OU2B-INSSEA-10
		4,4'-DDD	OU2B-FPSS11-10	NA	7.8	0.0078	31100	0.0311	0.25	5.7	0.0057	0.036	0.16	OU2B-INSSEA-10
		4,4'-DDE	*OU2B-FPSS11-10*	NA	*14.6*	*0.0146*	*31100*	*0.0311*	0.47	121	*0.121*	*0.036*	*3.4*	*OU2B-INSSEA-10*
		4,4'-DDT	OU2B-FPSS11-10	NA	*0.44*	*0.0004*	31100	0.0311	0.014	5.2	*0.0052*	0.036	0.14	OU2B-INSSEA-10
		DDTR [b]	**OU2B-FPSS11-10**			**0.036**			**1.15**					
		2,4'-DDD	OU2B-FPSS12-10	NA	0.68	0.00068	15900	0.0159	0.043					
		2,4'-DDE	OU2B-FPSS12-10	NA	0.85	0.00085	15900	0.0159	0.053					
		2,4'-DDT	OU2B-FPSS12-10	NA	*0.38*	*0.00038*	15900	0.0159	0.024					
		4,4'-DDD	OU2B-FPSS12-10	NA	1.3	0.0013	15900	0.0159	0.082					
		4,4'-DDE	OU2B-FPSS12-10	NA	0.95	0.00095	15900	0.0159	0.060					
		4,4'-DDT	OU2B-FPSS12-10	NA	1.8	0.0018	15900	0.0159	0.113					
		DDTR [b]	**OU2B-FPSS12-10**			**0.0060**			**0.37**					
	AVEREAGE DDTR (Southeast) [c]					**0.021**			**0.76**		**0.142**		**3.95**	**OU2B-INSSEA-10**
Insects (Southwest) 1994 - Composite (d)	3	DDTR	OSG0701-0694	1439.8	1660.15	1.66	45600 (e)	0.046	31.1	NA	0.13	0.0378	3.44	OIN0303
			OSG0701FD-0694	1880.5	NA	NA								
			OSG0702-0694	738.5	NA	0.74								
			OSG0703-0694	1896.4	NA	1.90								
		DDTR	**OSG07**			**1.43**			**31.1**		**0.13**		**3.44**	**OIN0303**

Notes:
*Data pairs represent a 400-foot forage area.
(a) Duplicate samples were averaged together to obtain a representative concentration.
(b) DDTR is the sum of 2,4'- and 4,4'-isomers of DDD, DDE, and DDT
(c) Average DDTR concentration of all samples in area.
(d) Composite insect DDTr values from 1994 multiplied by 1.97 to obtain representative DDTR concentrations.
Terrestrial insects from 1994 include crawling, climbing, and flying insects composited together. This sample will be combined with the complete dataset for the purposes of BAF analysis; however, the sample will not be included when considering individual types of insects.
(e) Average TOC in all basin samples.
Concentrations in *italics* were non-detect for DDT isomer. A value of 1/2 the detection limit used as a representative concentration.
NA = Not Applicable
A = Spiders
B = Flying Insects
C = Crawling Insects

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FIGURE D-1a

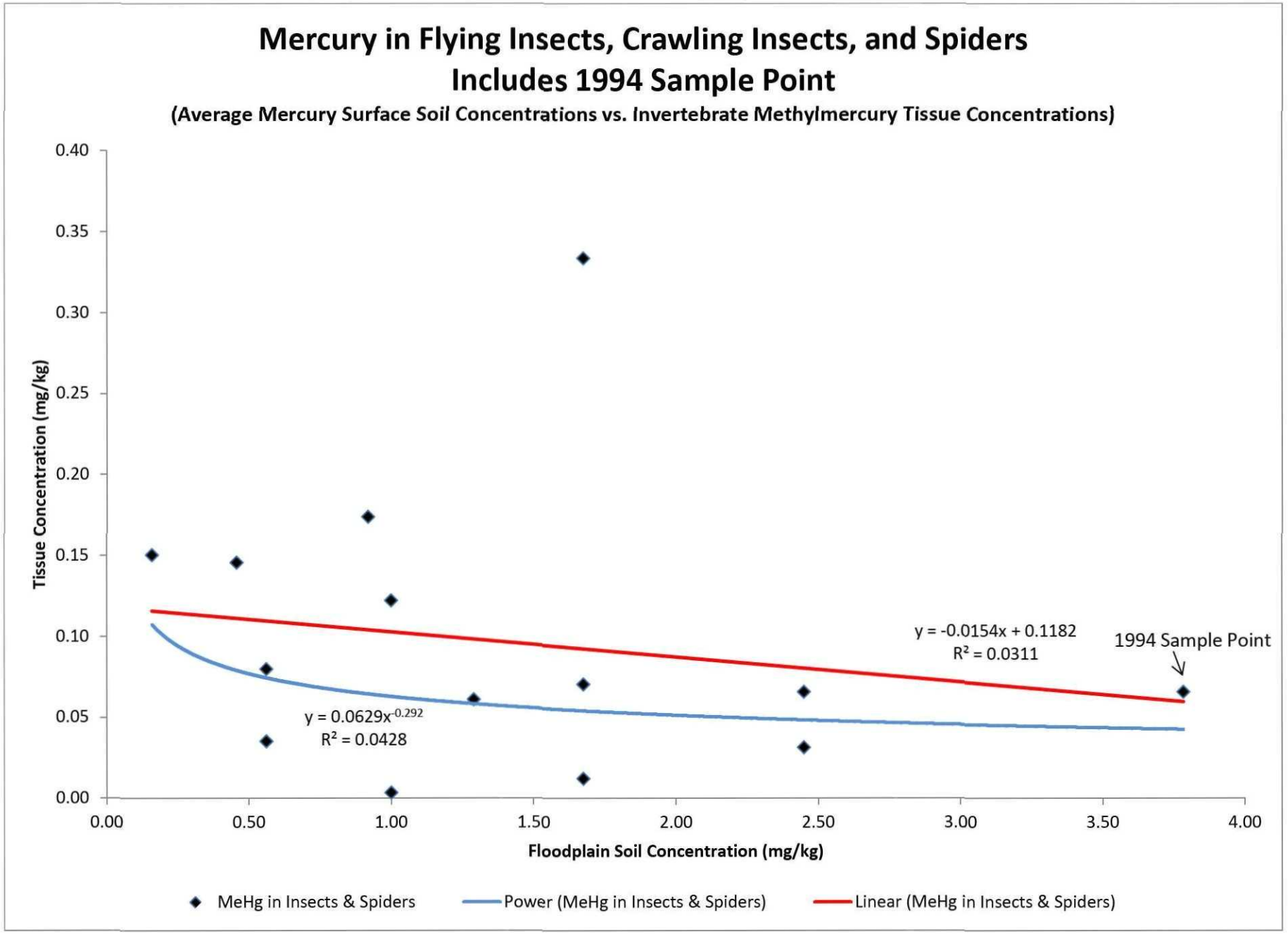

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FIGURE D-1b

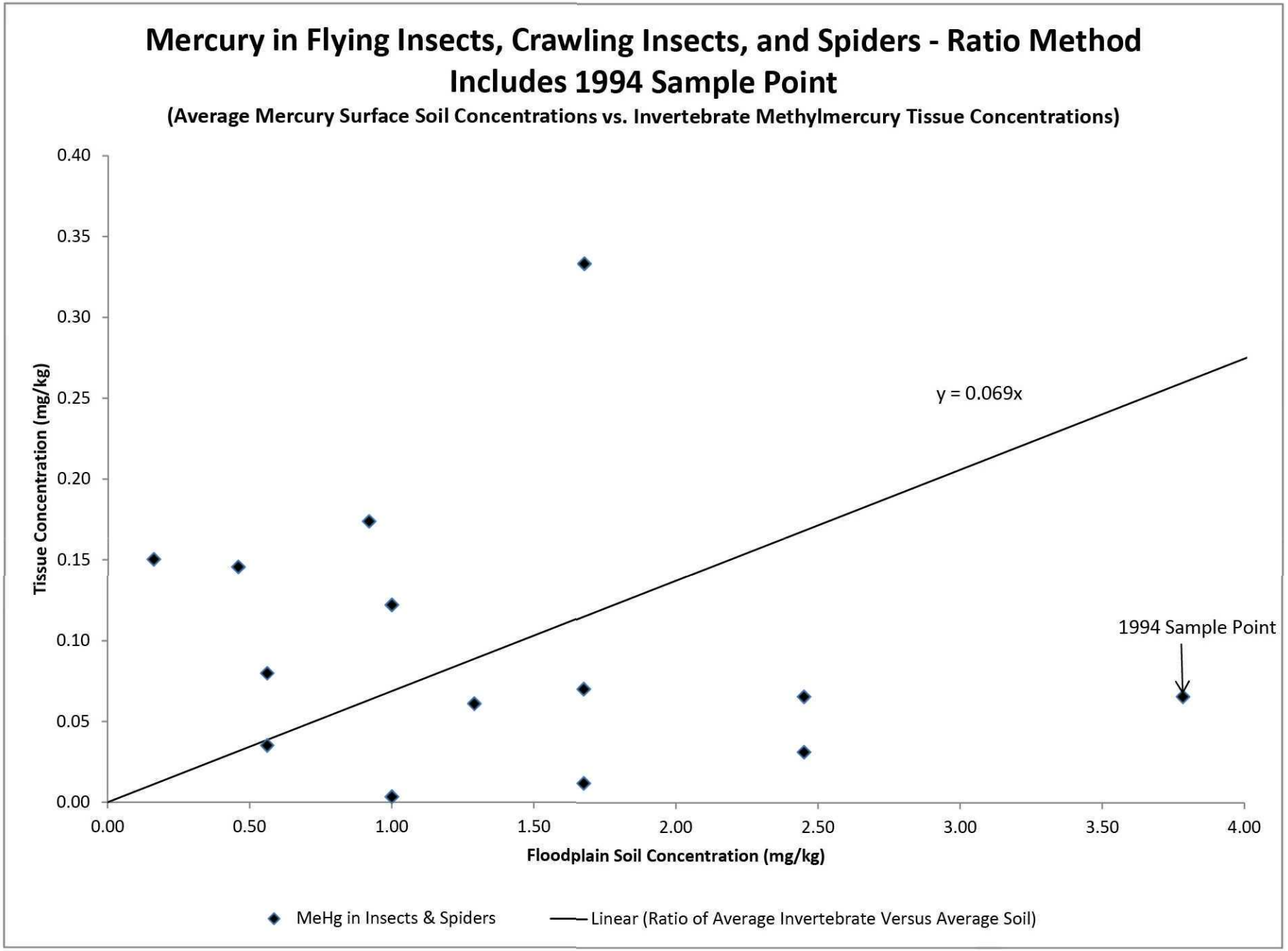

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FIGURE D-1c

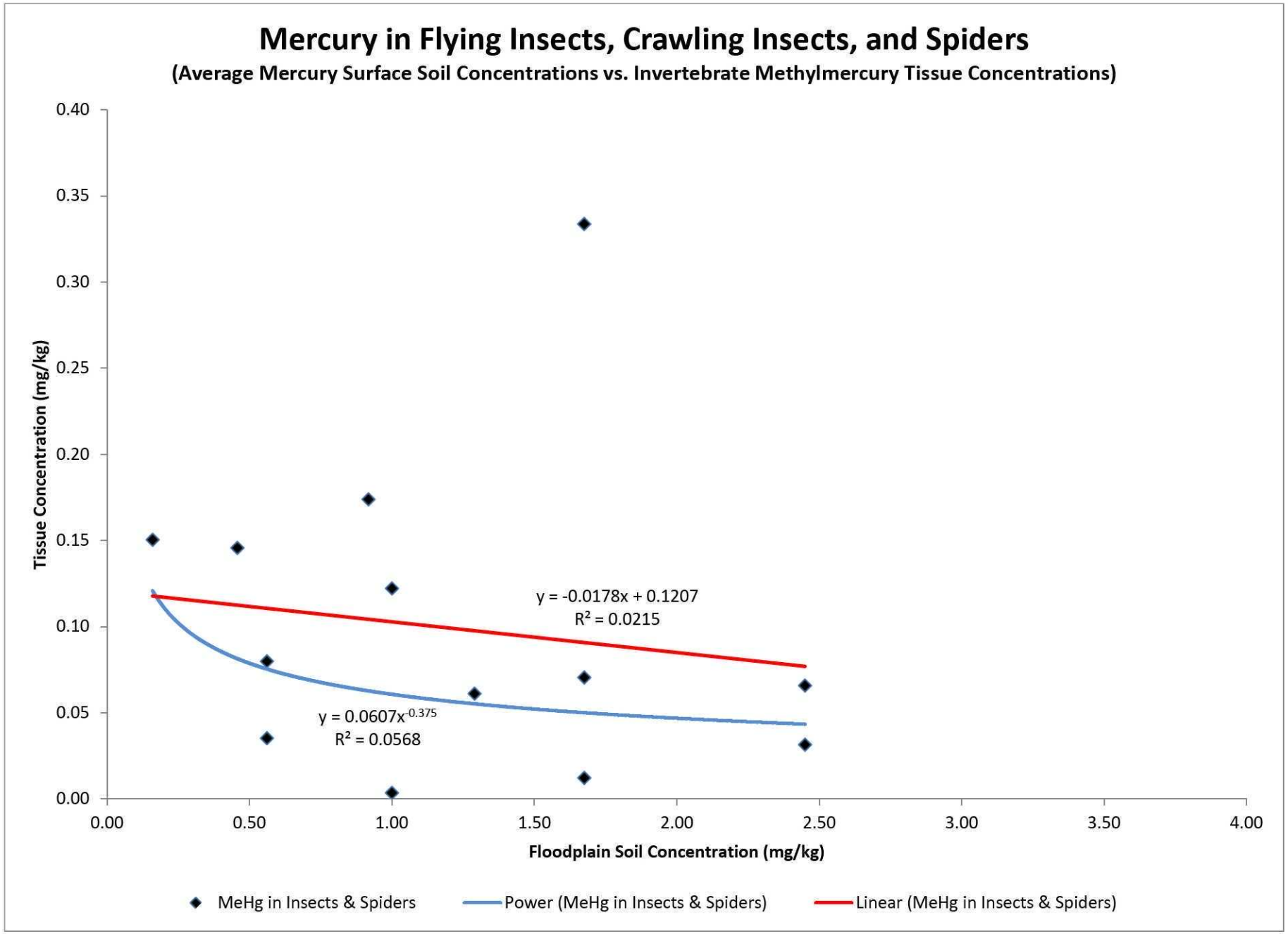

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FIGURE D-1d

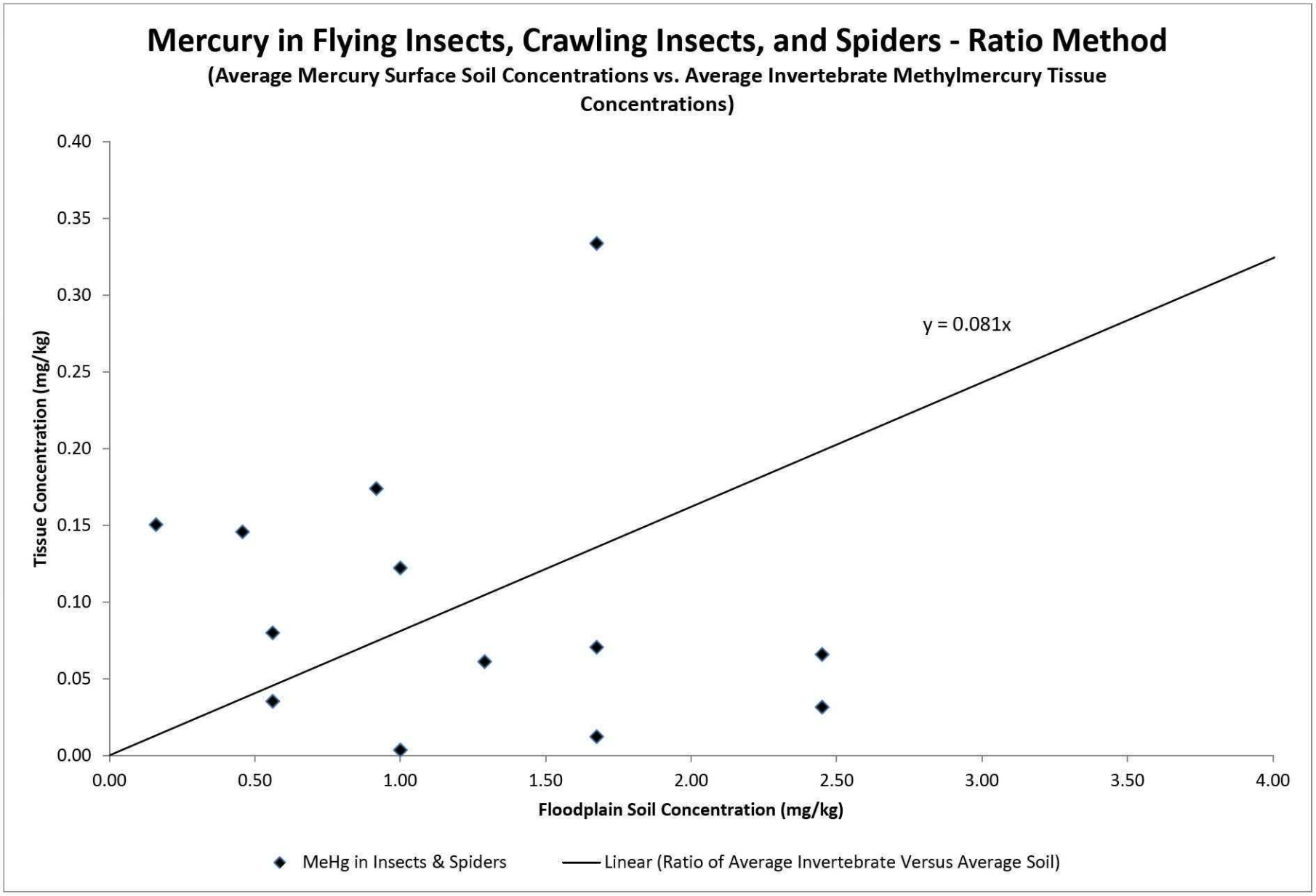

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FIGURE D-2a

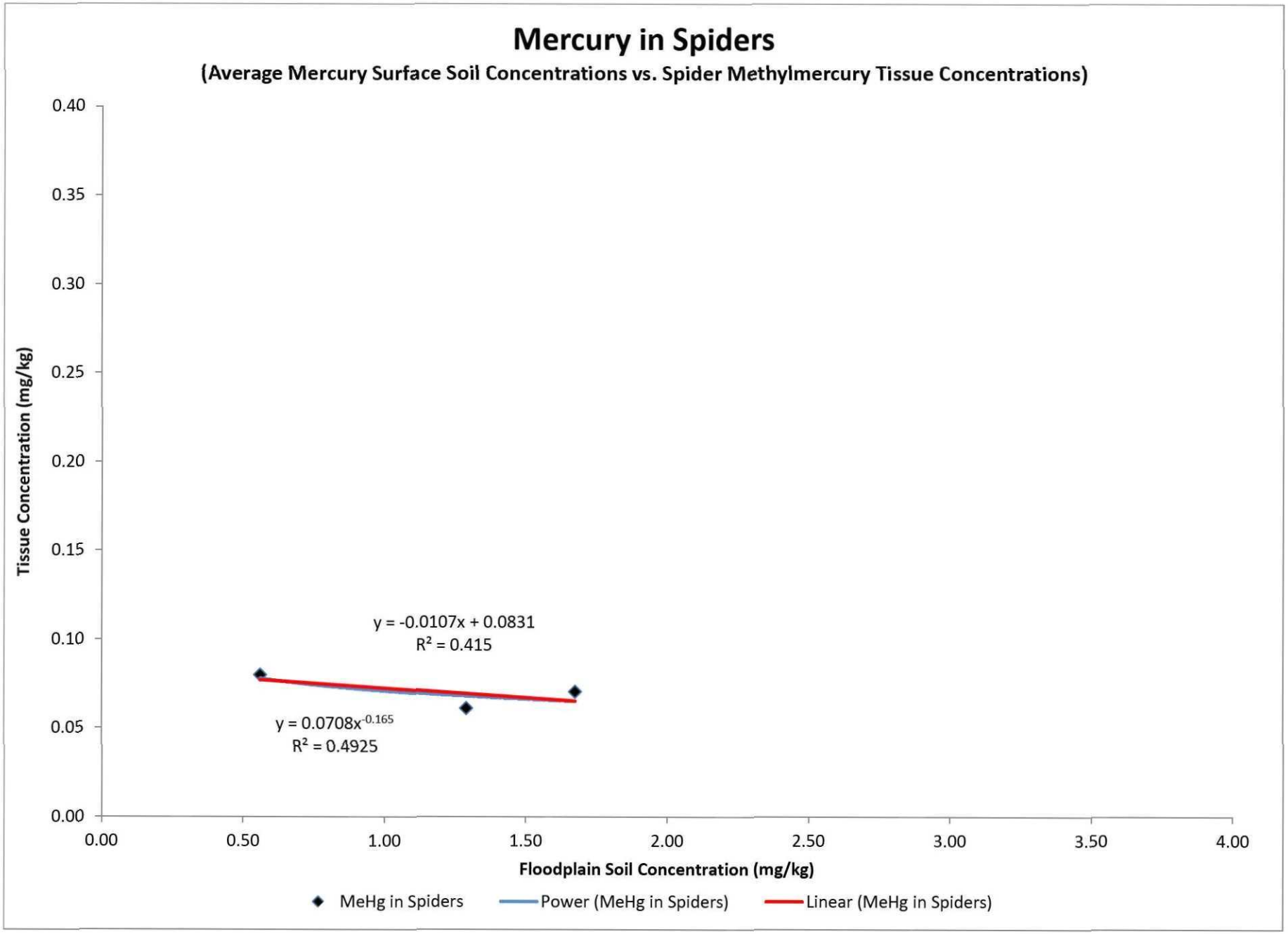

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FIGURE D-2b

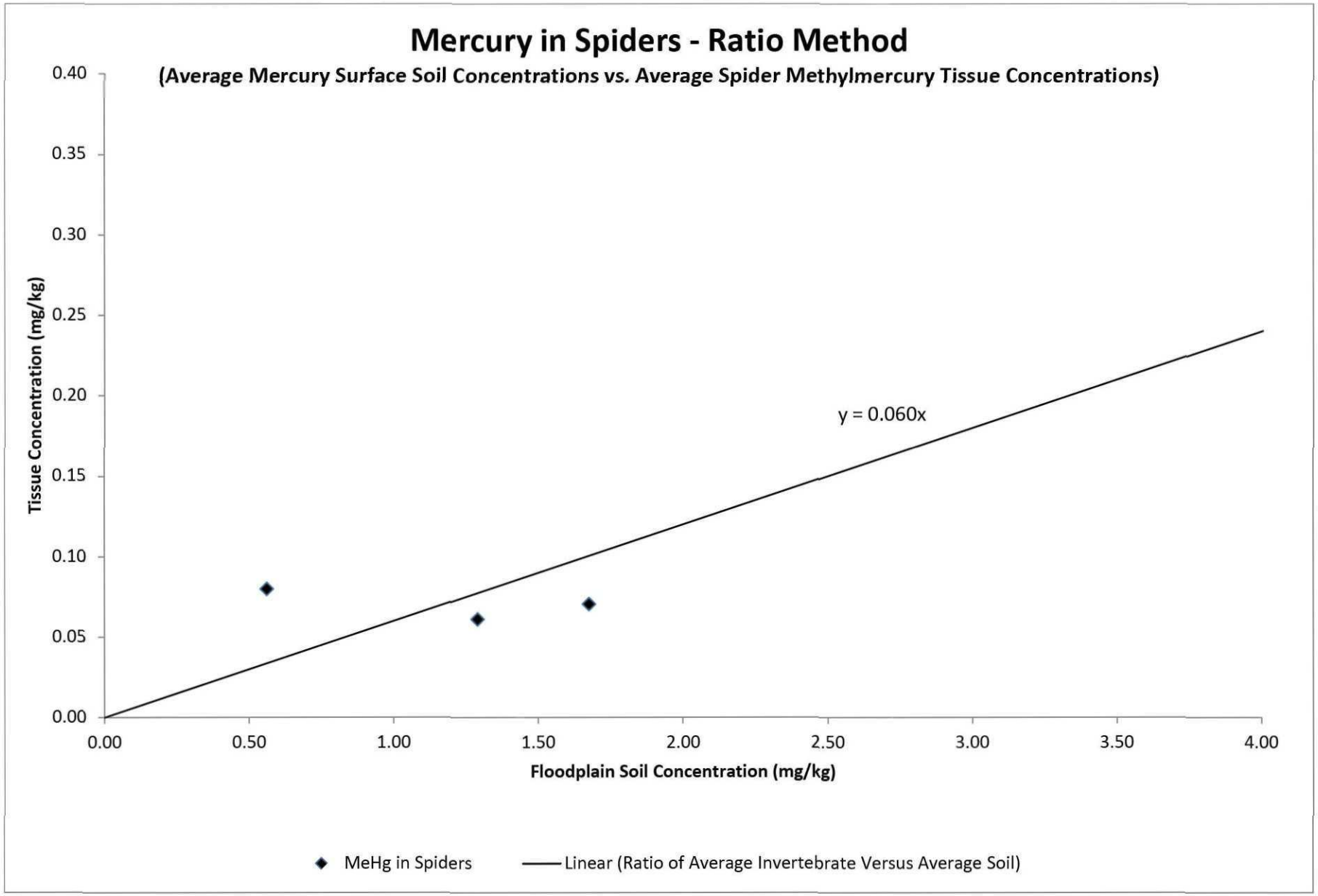

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FIGURE D-3a

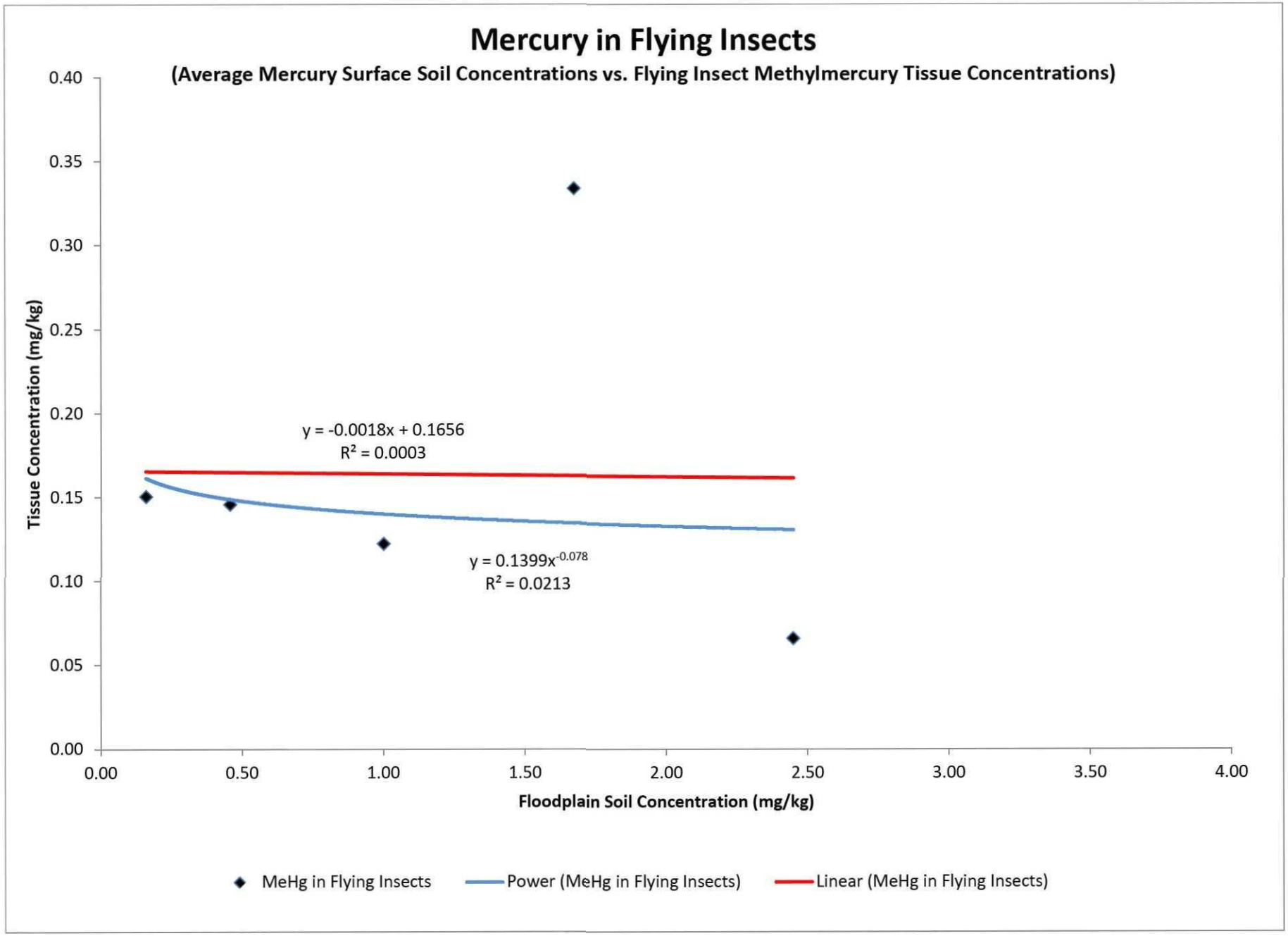

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FIGURE D-3b

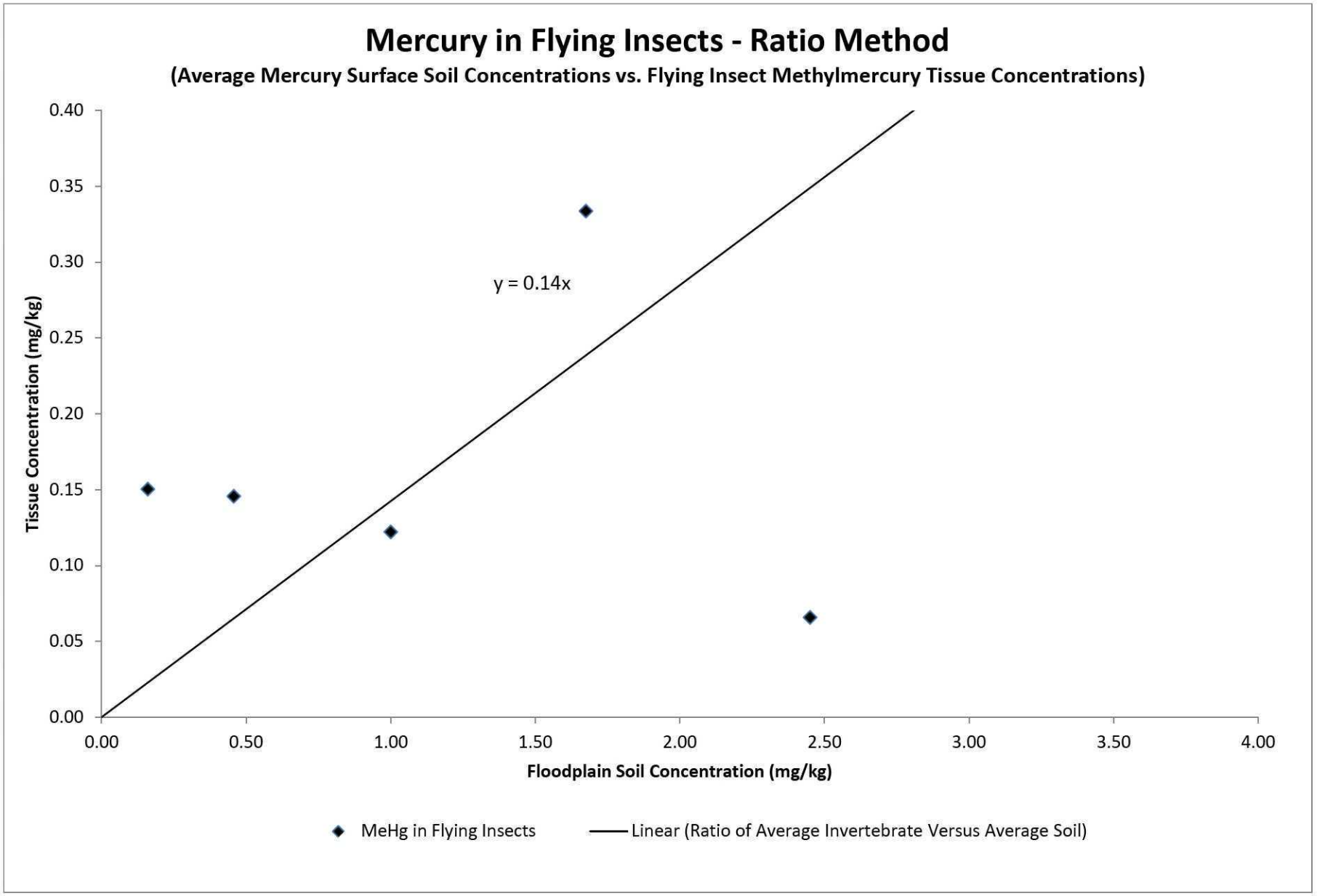

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FIGURE D-4a

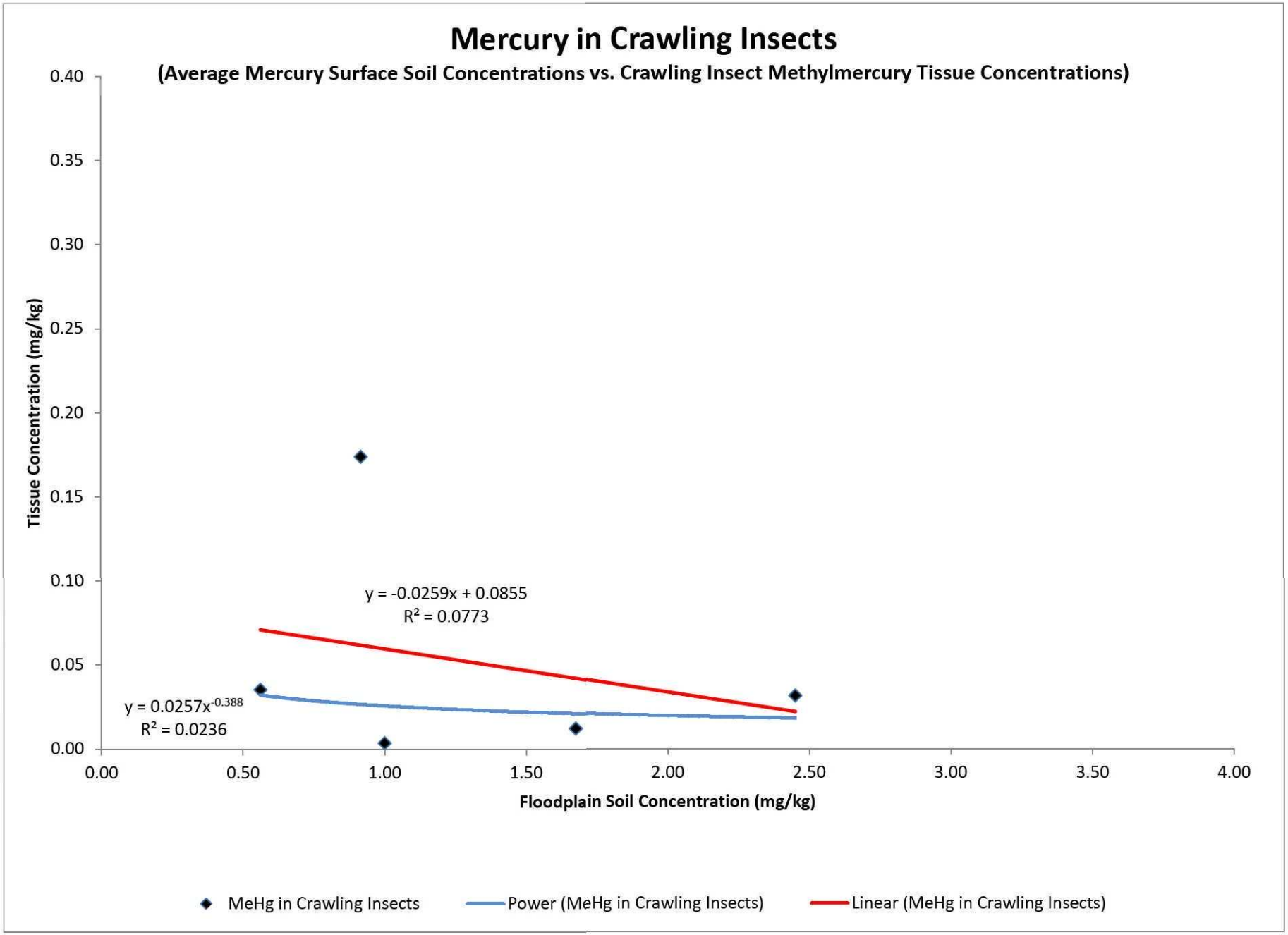

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FIGURE D-4b

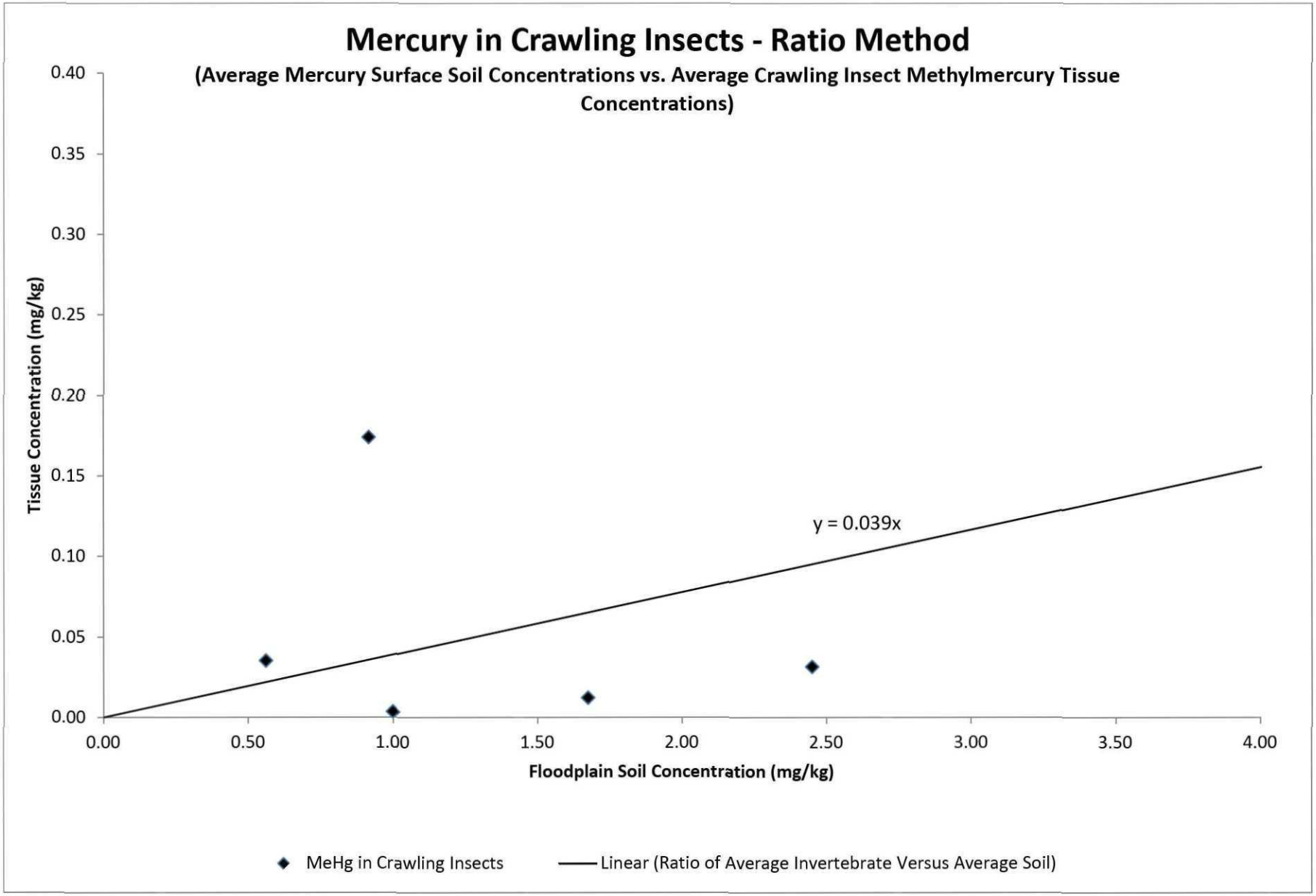

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FIGURE D-5a

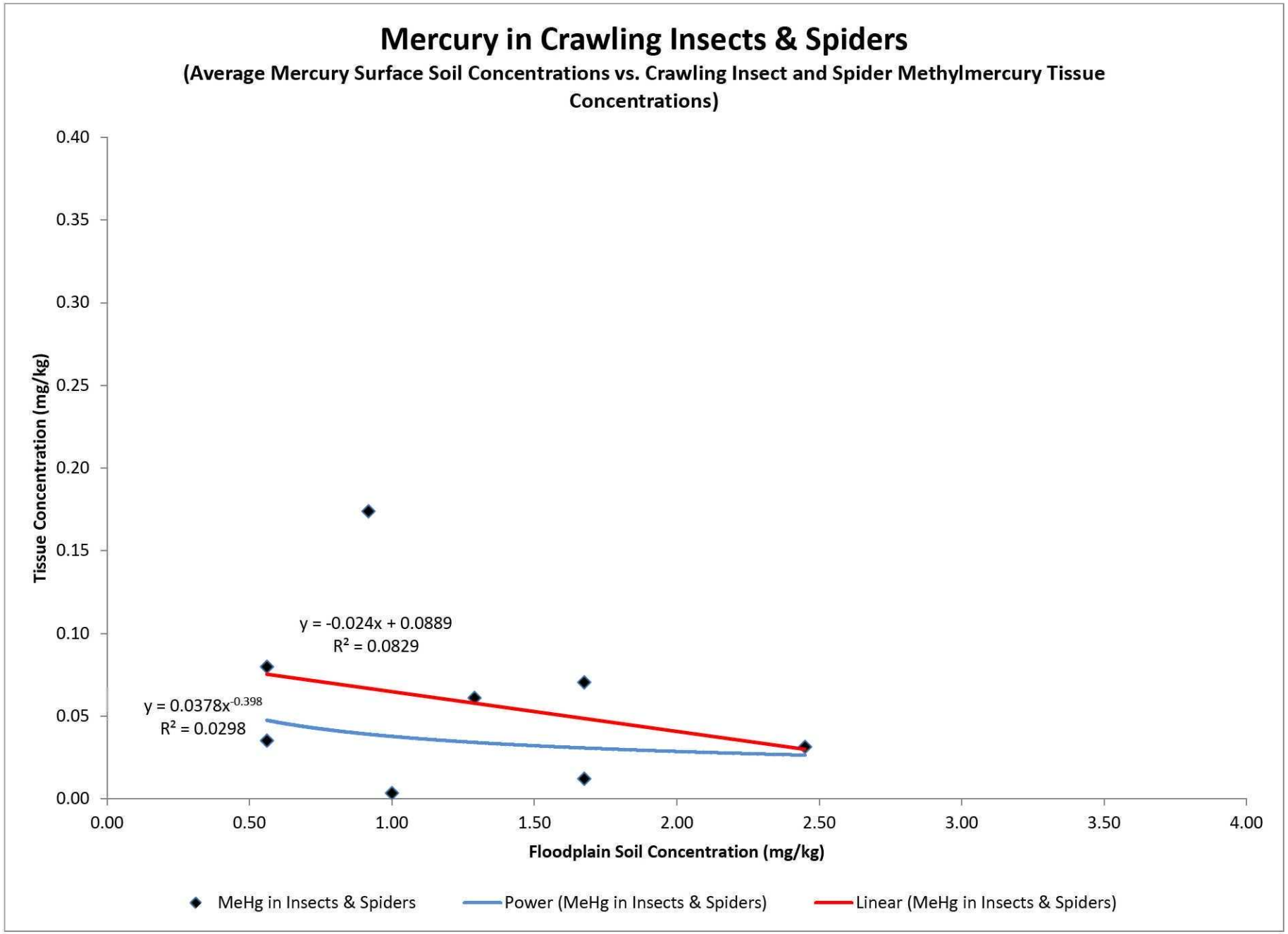

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FIGURE D-5b

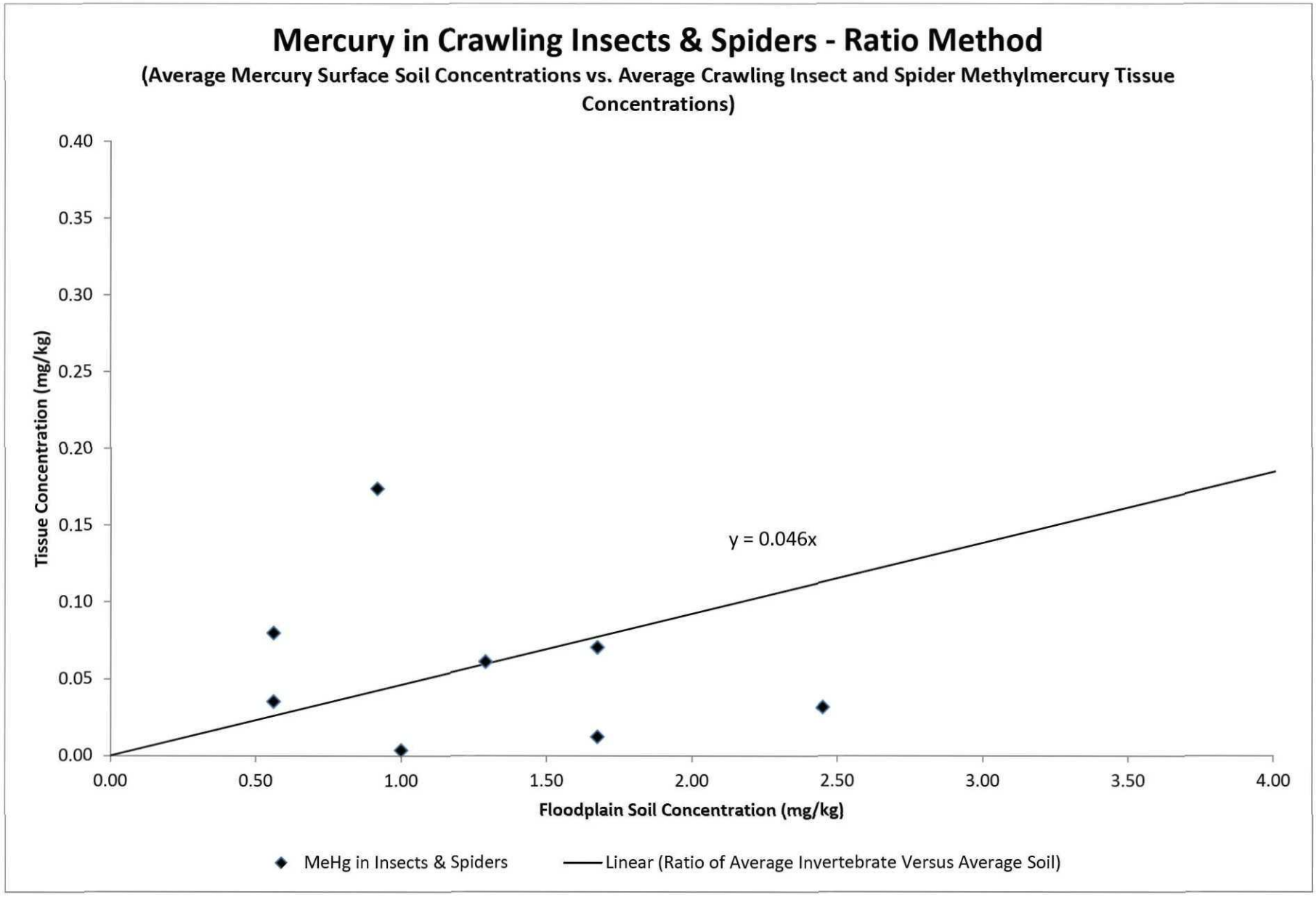

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FIGURE D-6a

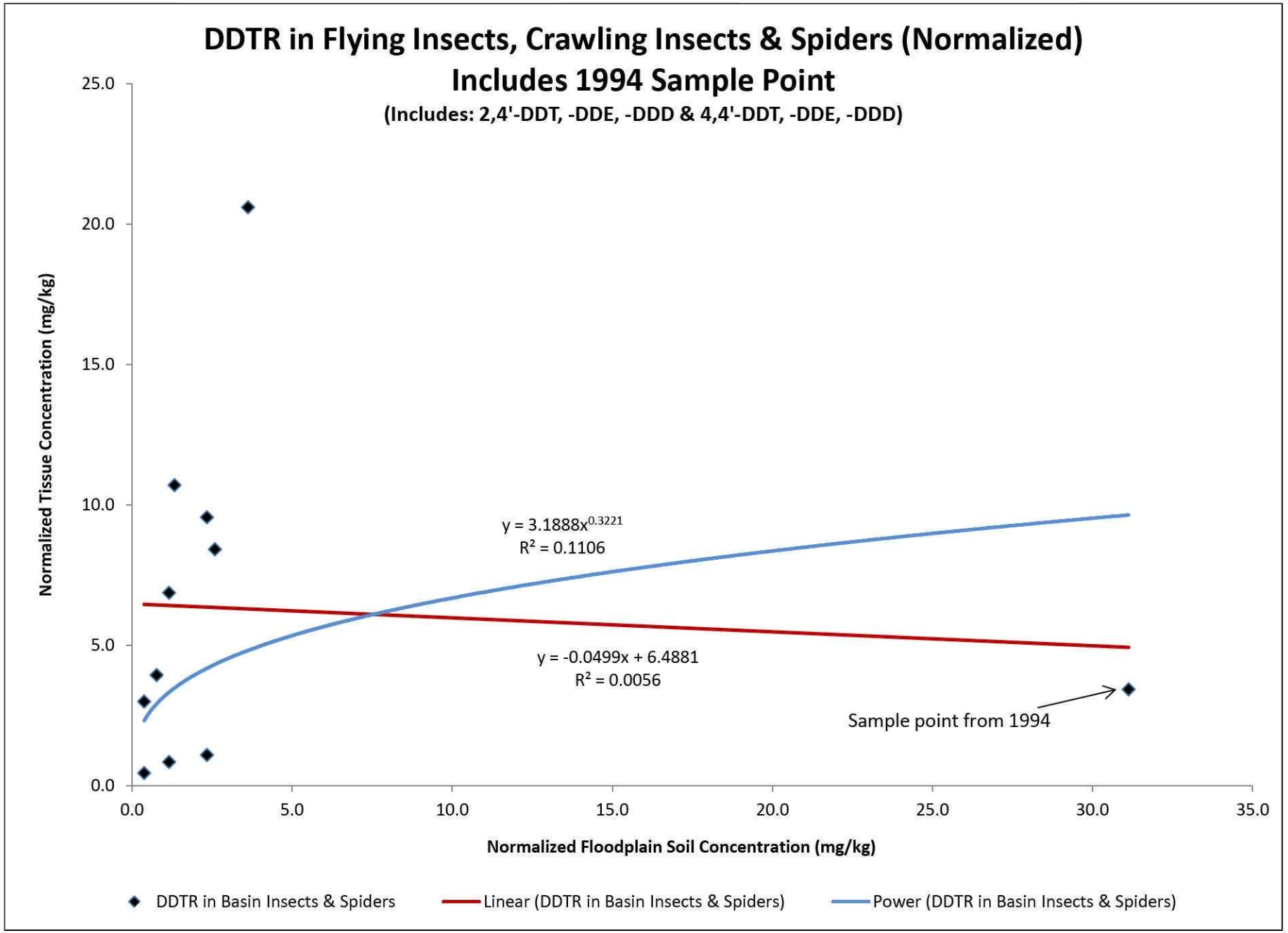

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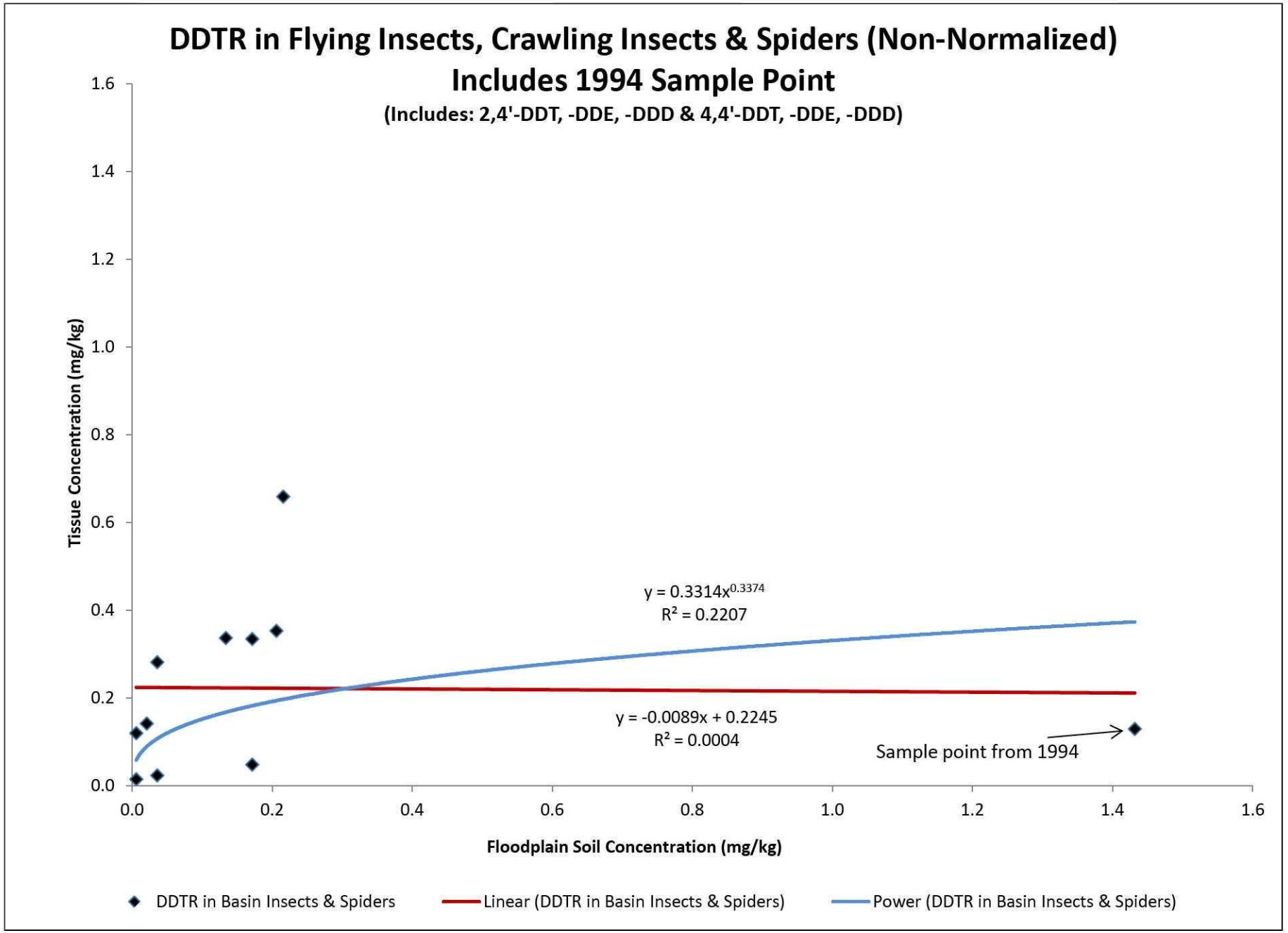
FIGURE D-6b



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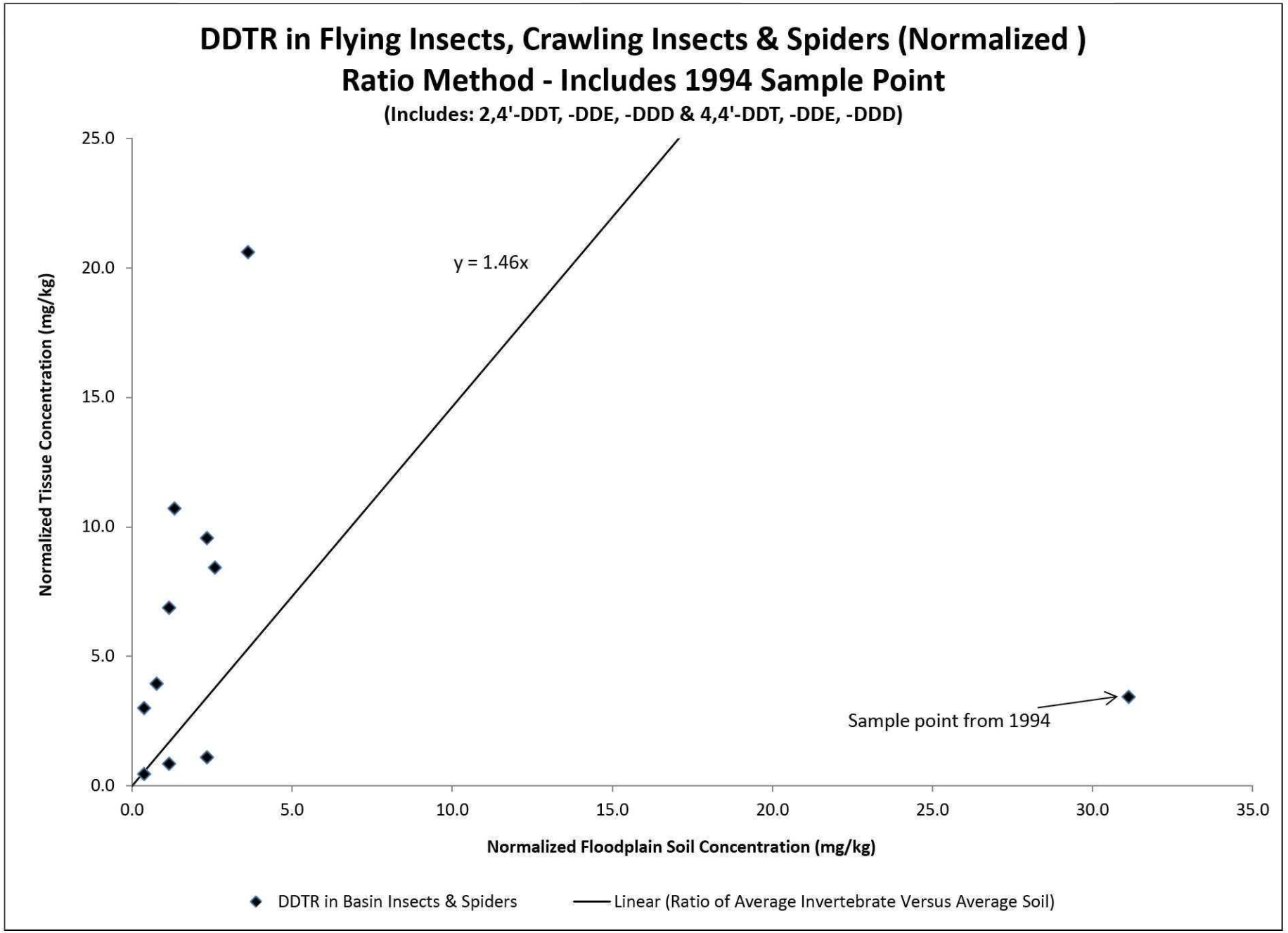
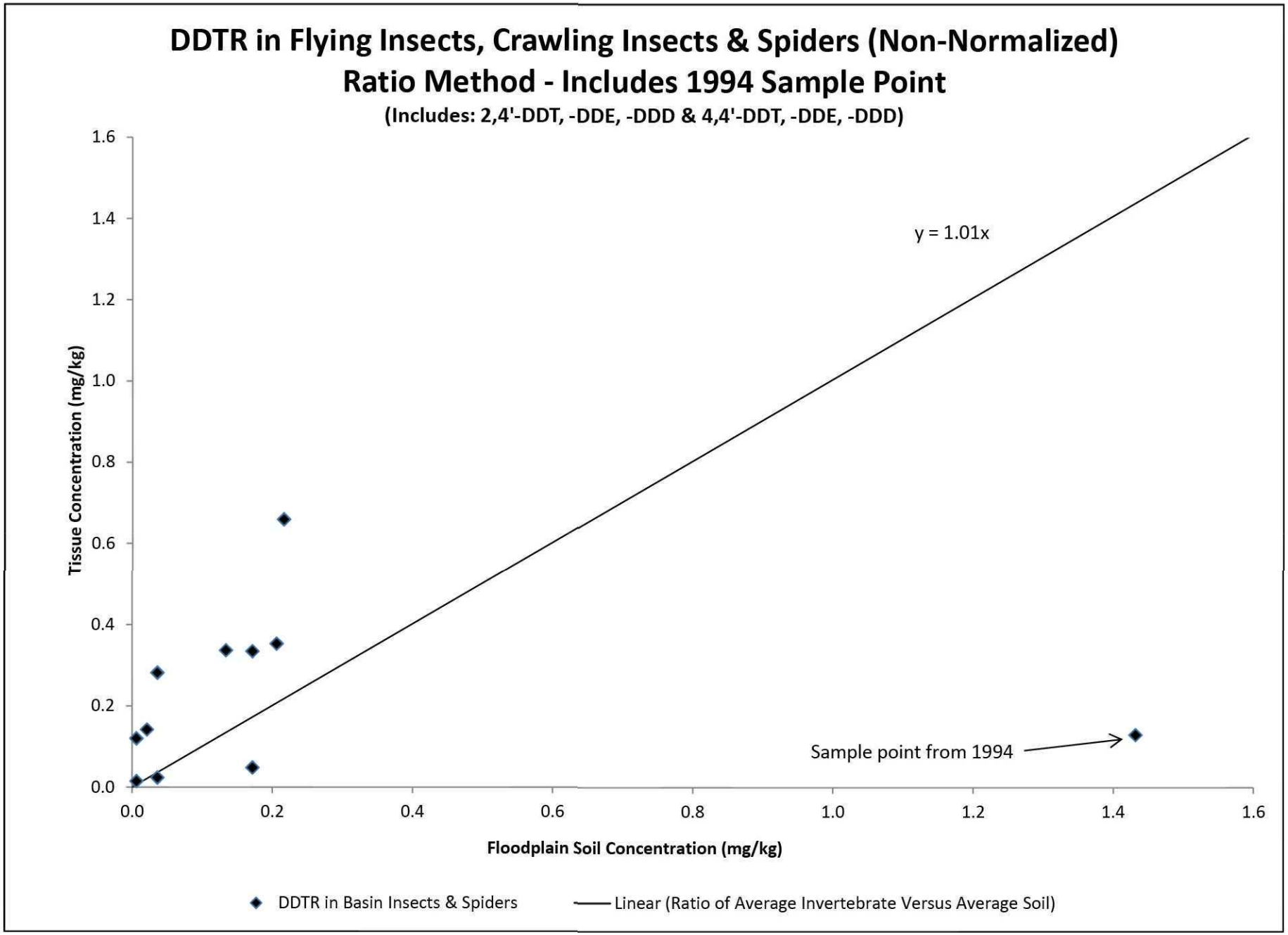
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-6c



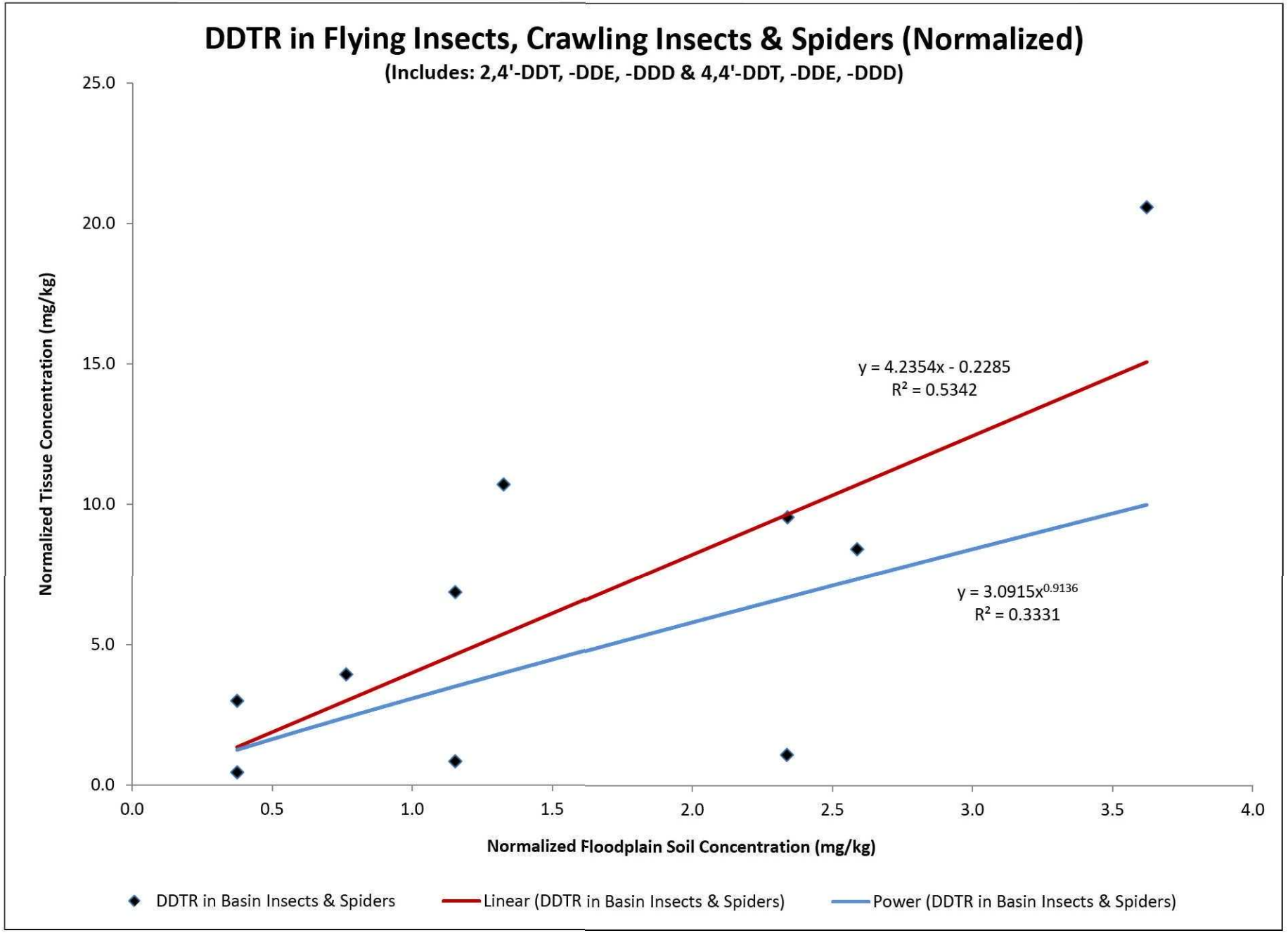
PREPARED BY/DATE: MKB 1/23/12
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-6d



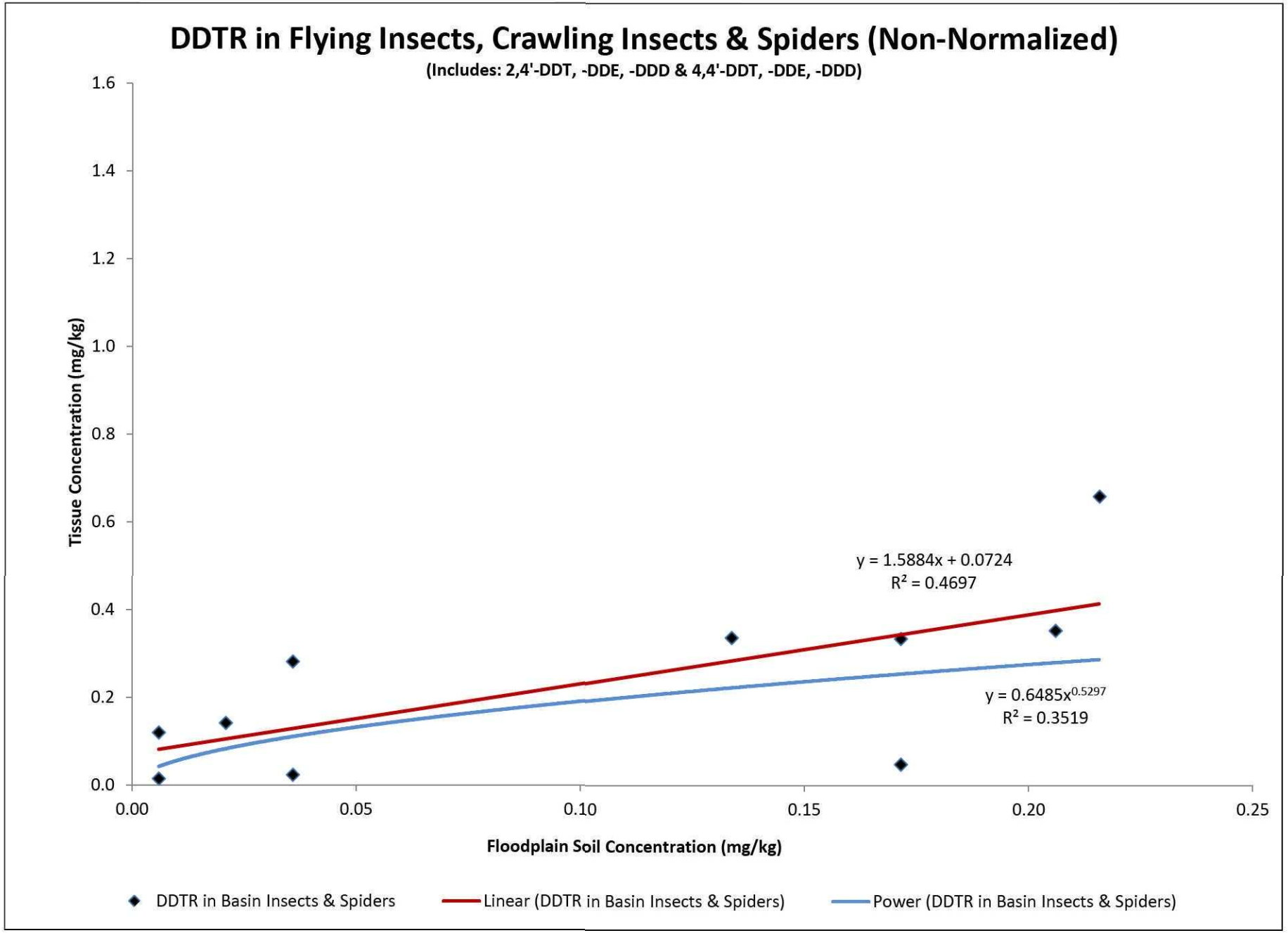
PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-7a



PREPARED BY/DATE: MKB 1/23/12
CHECKED BY/DATE: NSR 1/24/12

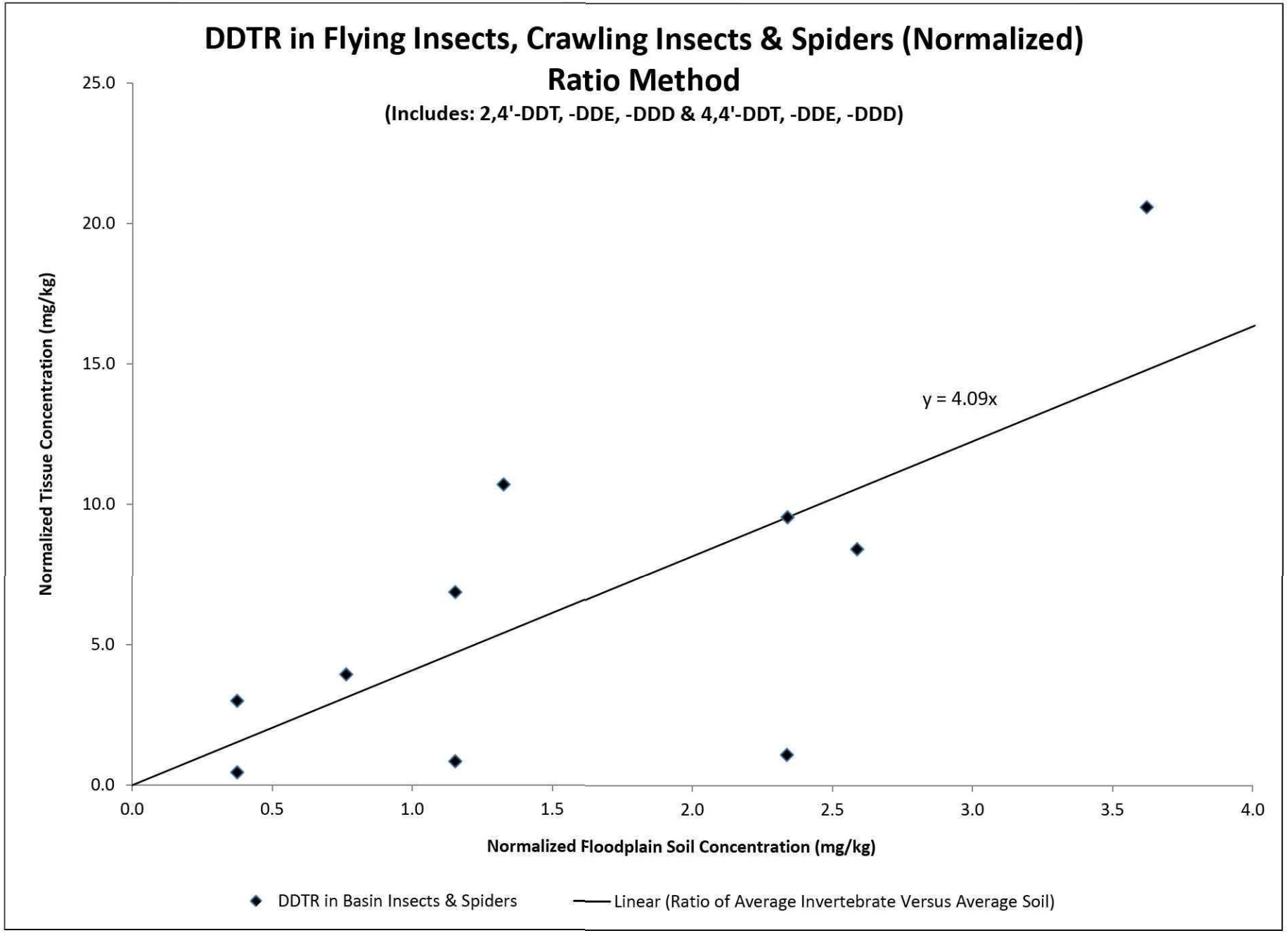
FIGURE D-7b



PREPARED BY/DATE: MKB 01/23/12

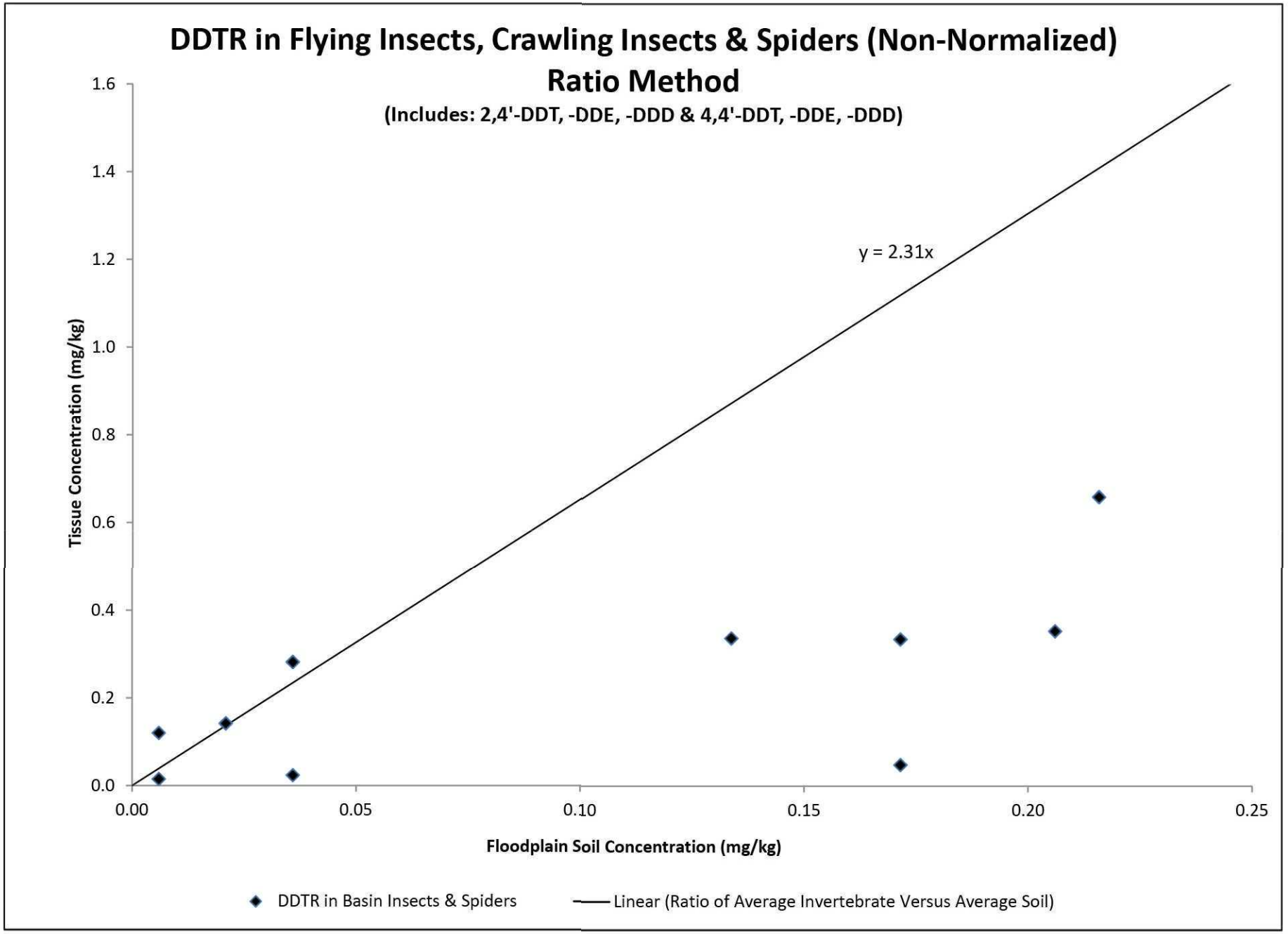
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-7c



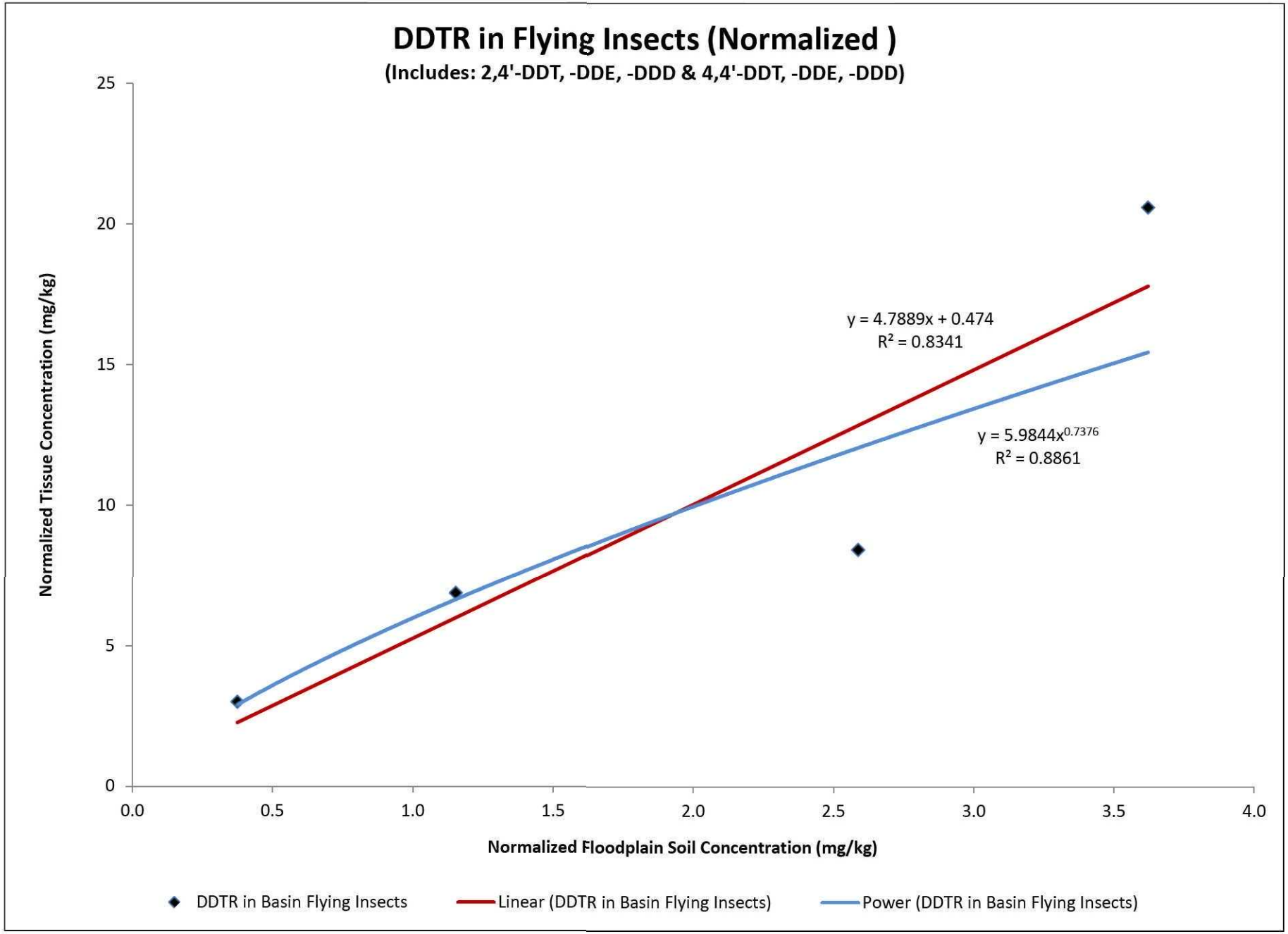
PREPARED BY/DATE: MKB 1/23/12
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-7d



PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

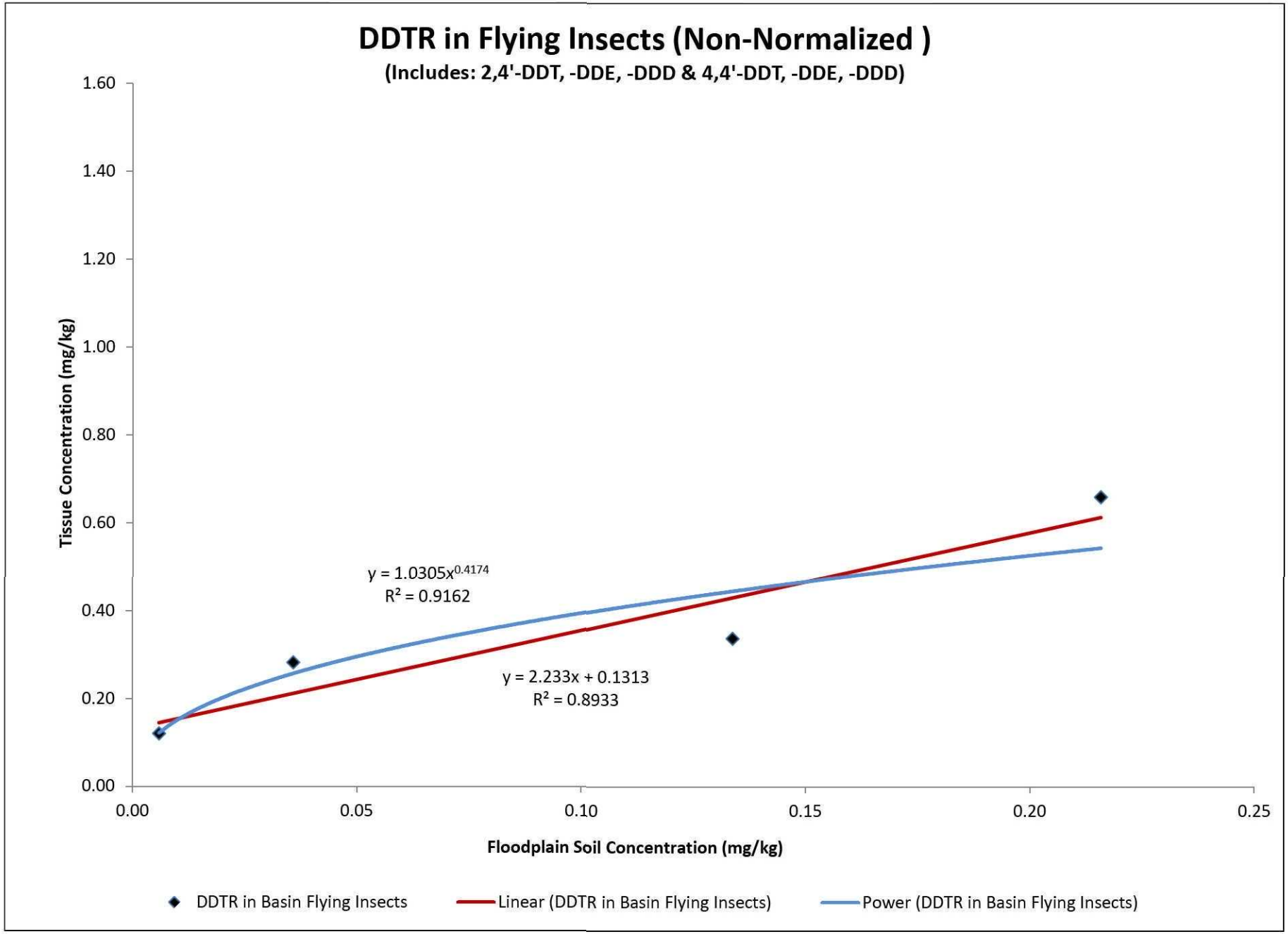
FIGURE D-8a



PREPARED BY/DATE: MKB 01/23/12

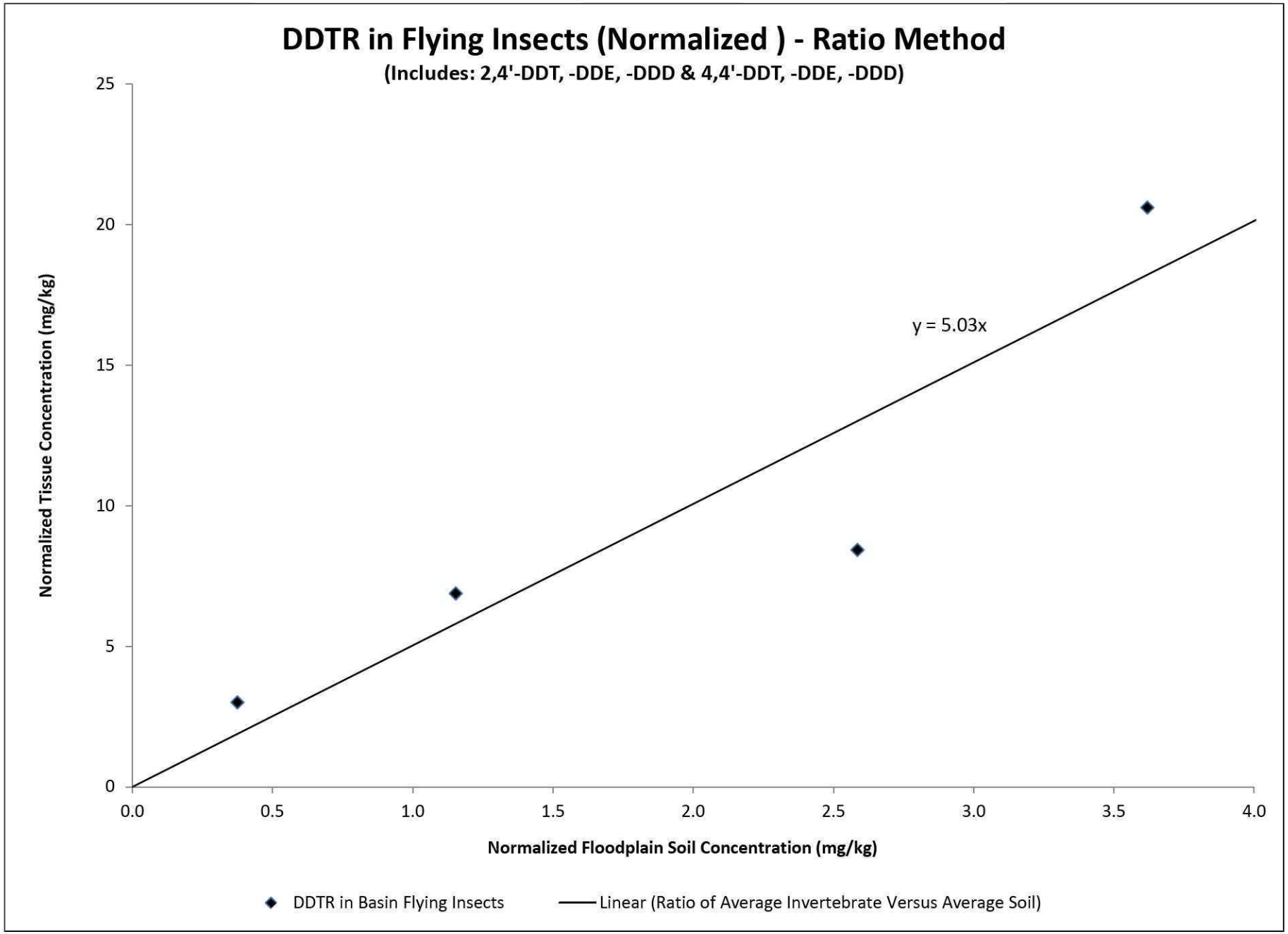
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-8b



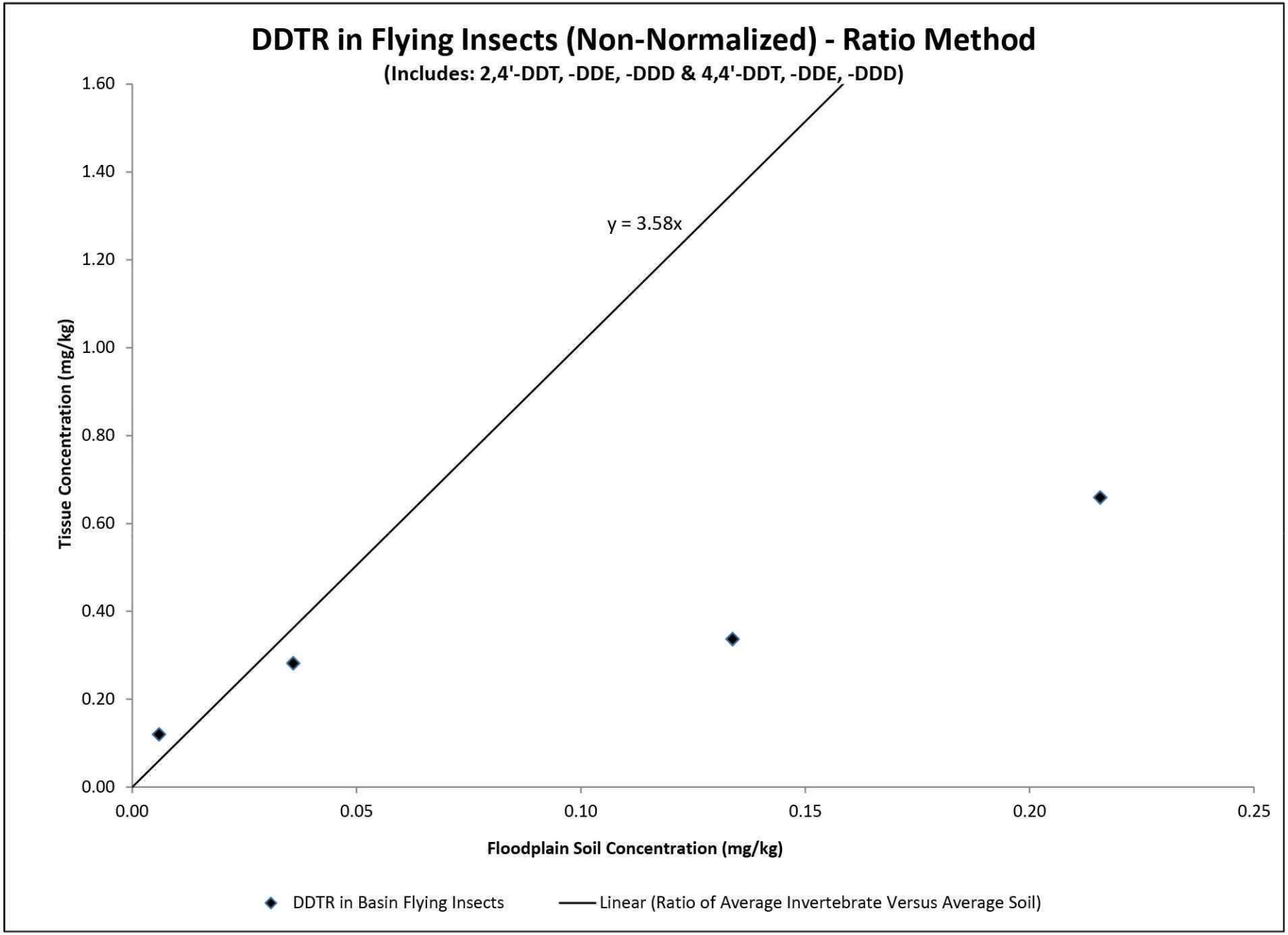
PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-8c



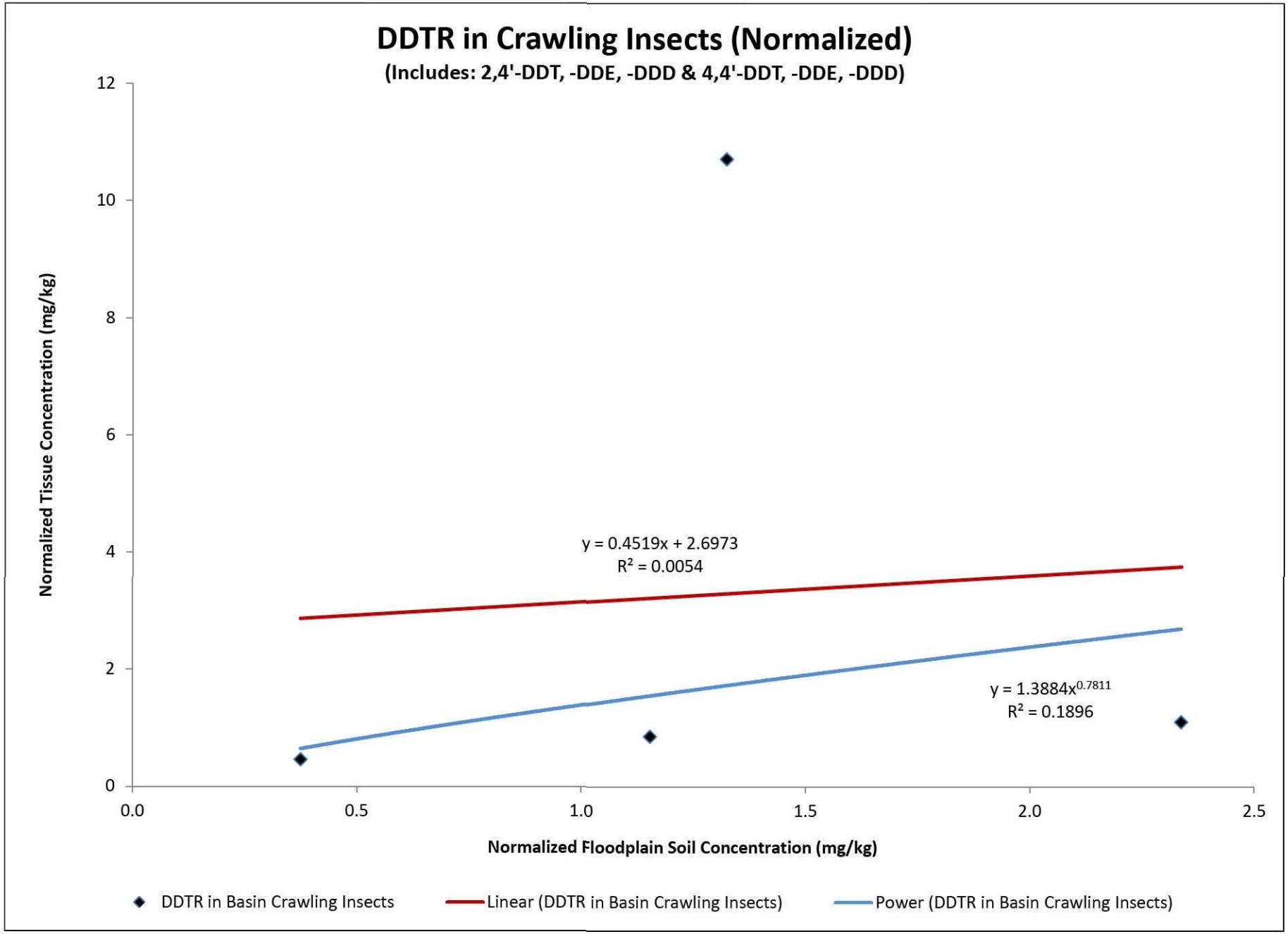
PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-8d



PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

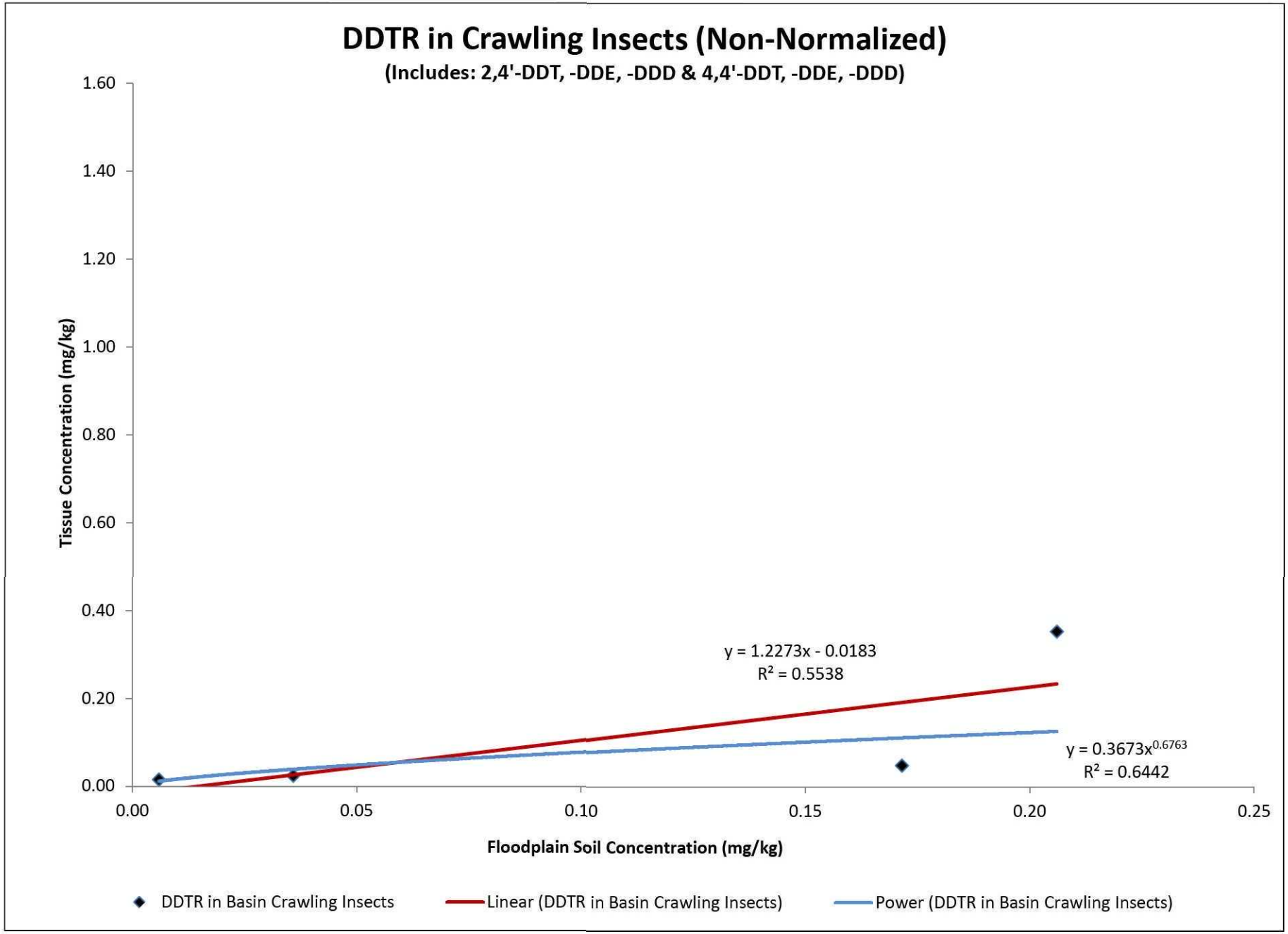
FIGURE D-9a



PREPARED BY/DATE: MKB 01/23/12

CHECKED BY/DATE: NSR 1/24/12

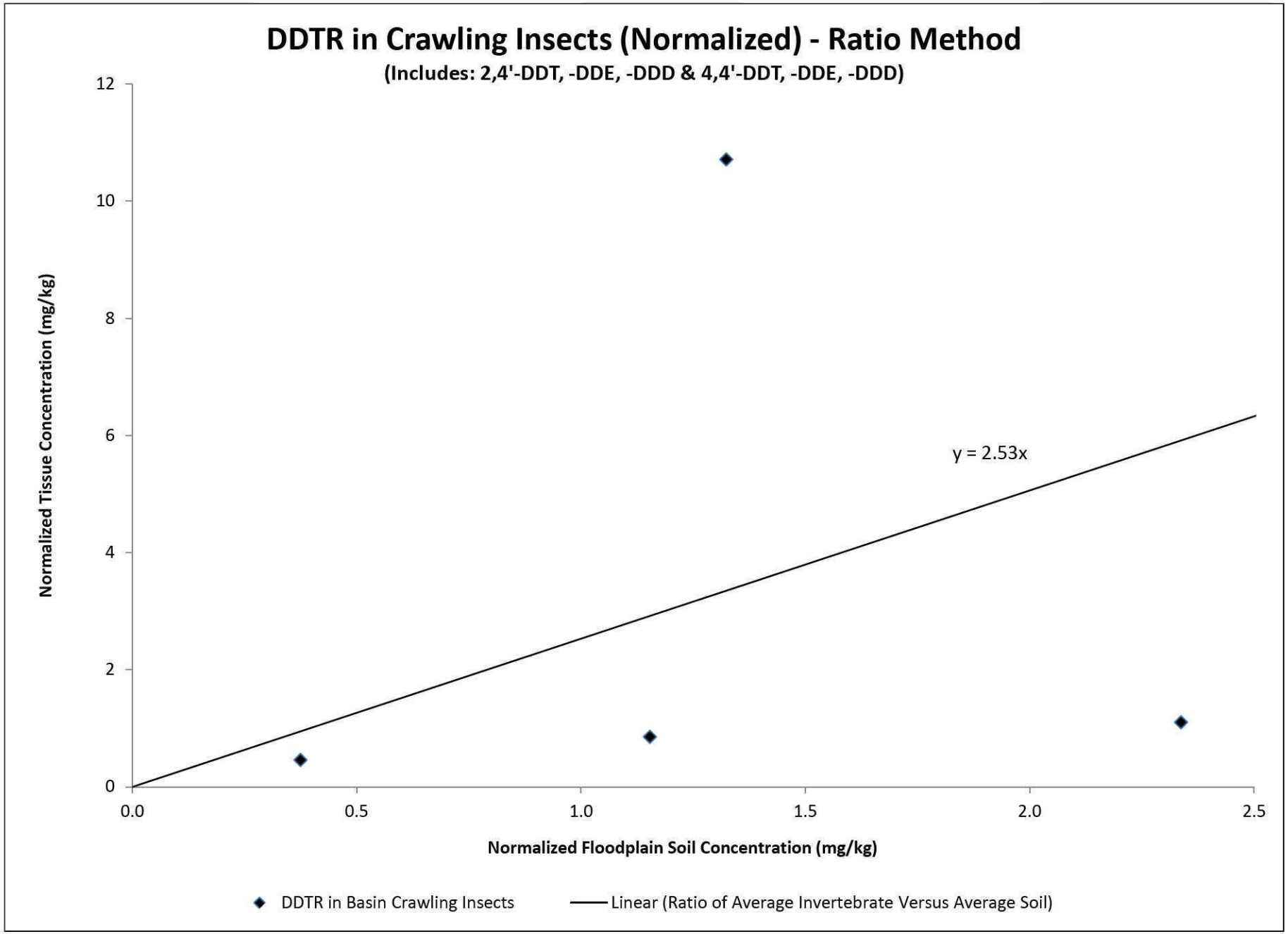
FIGURE D-9b



PREPARED BY/DATE: MKB 01/23/12

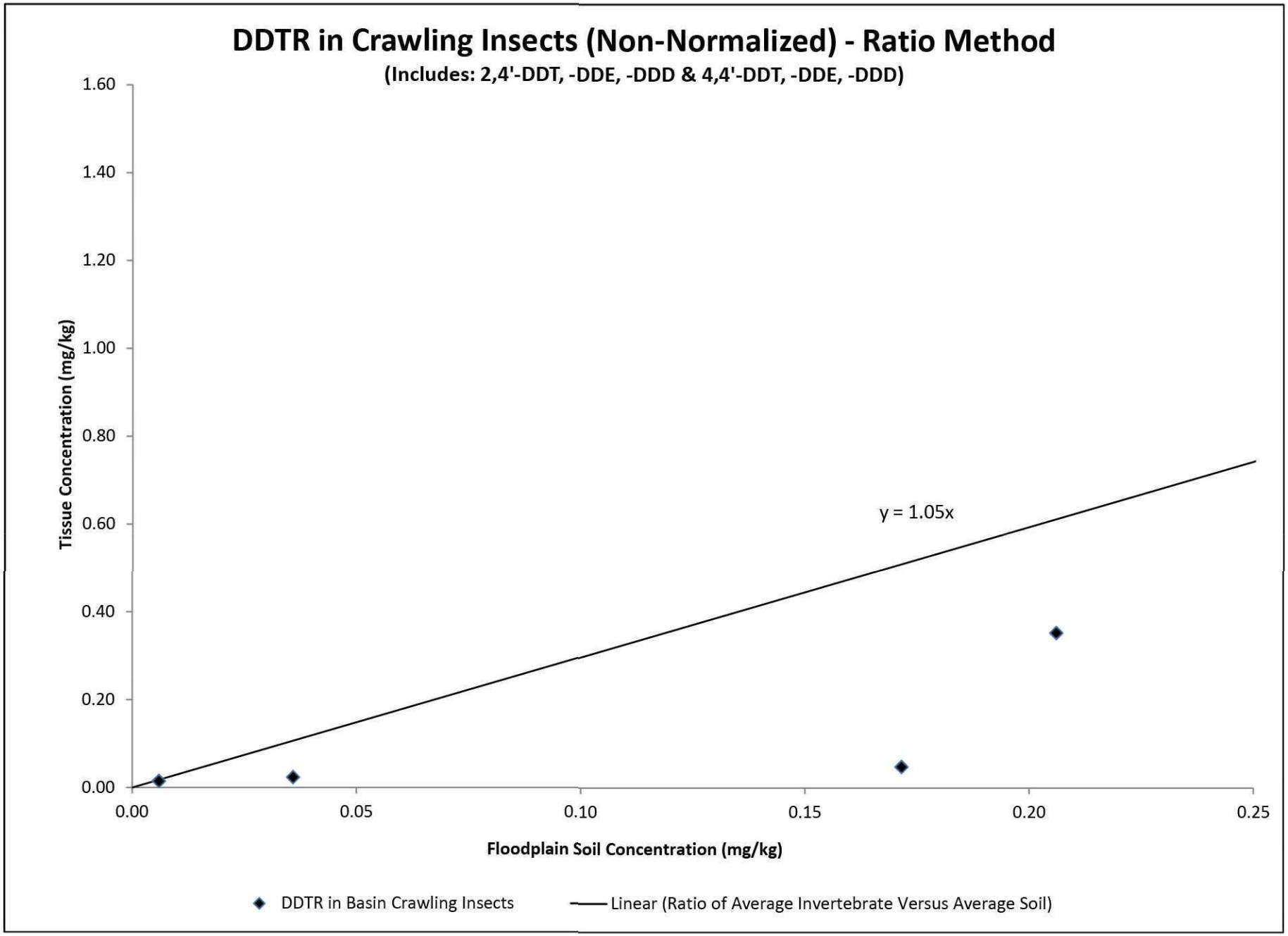
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-9c



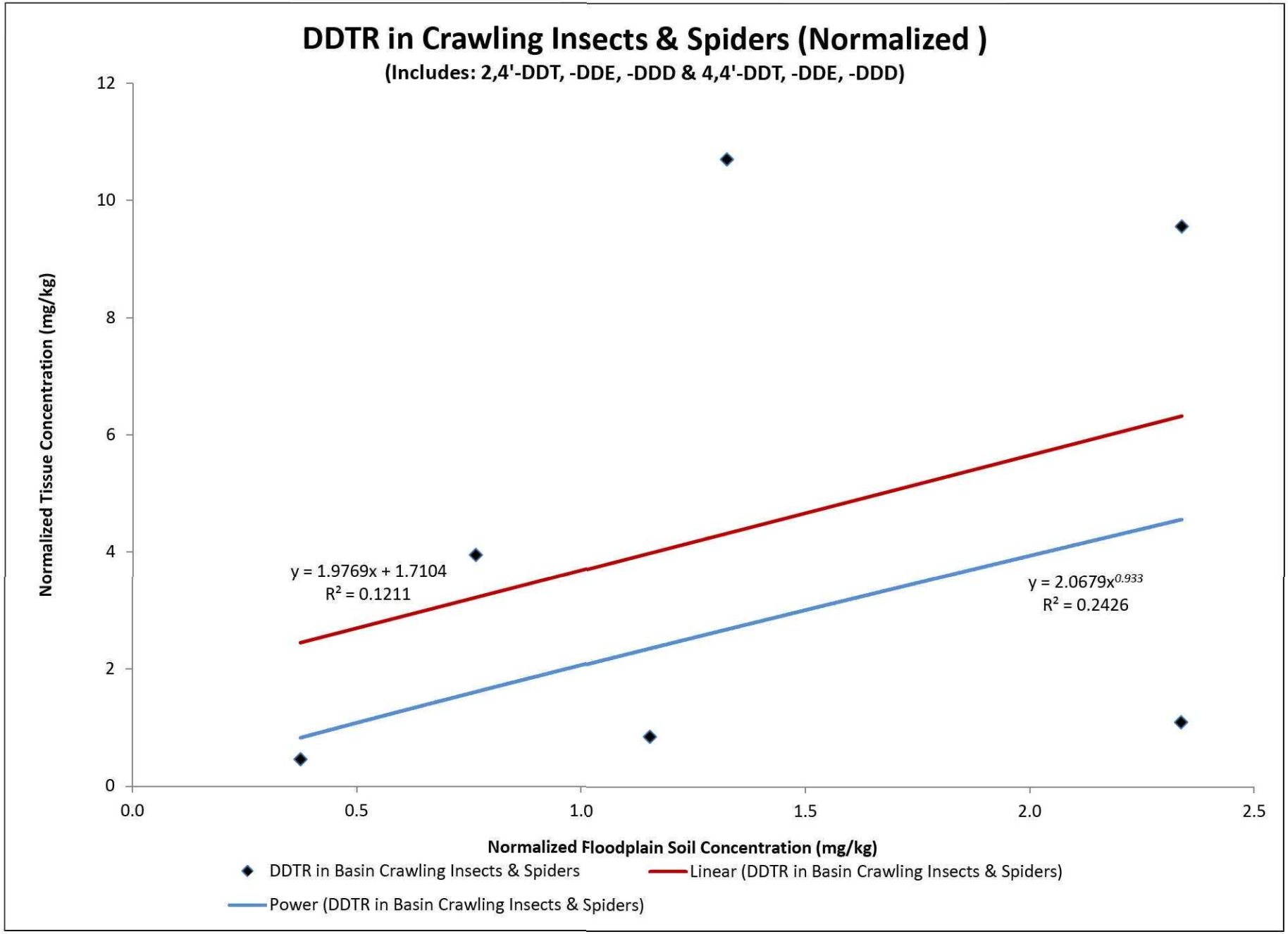
PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-9d



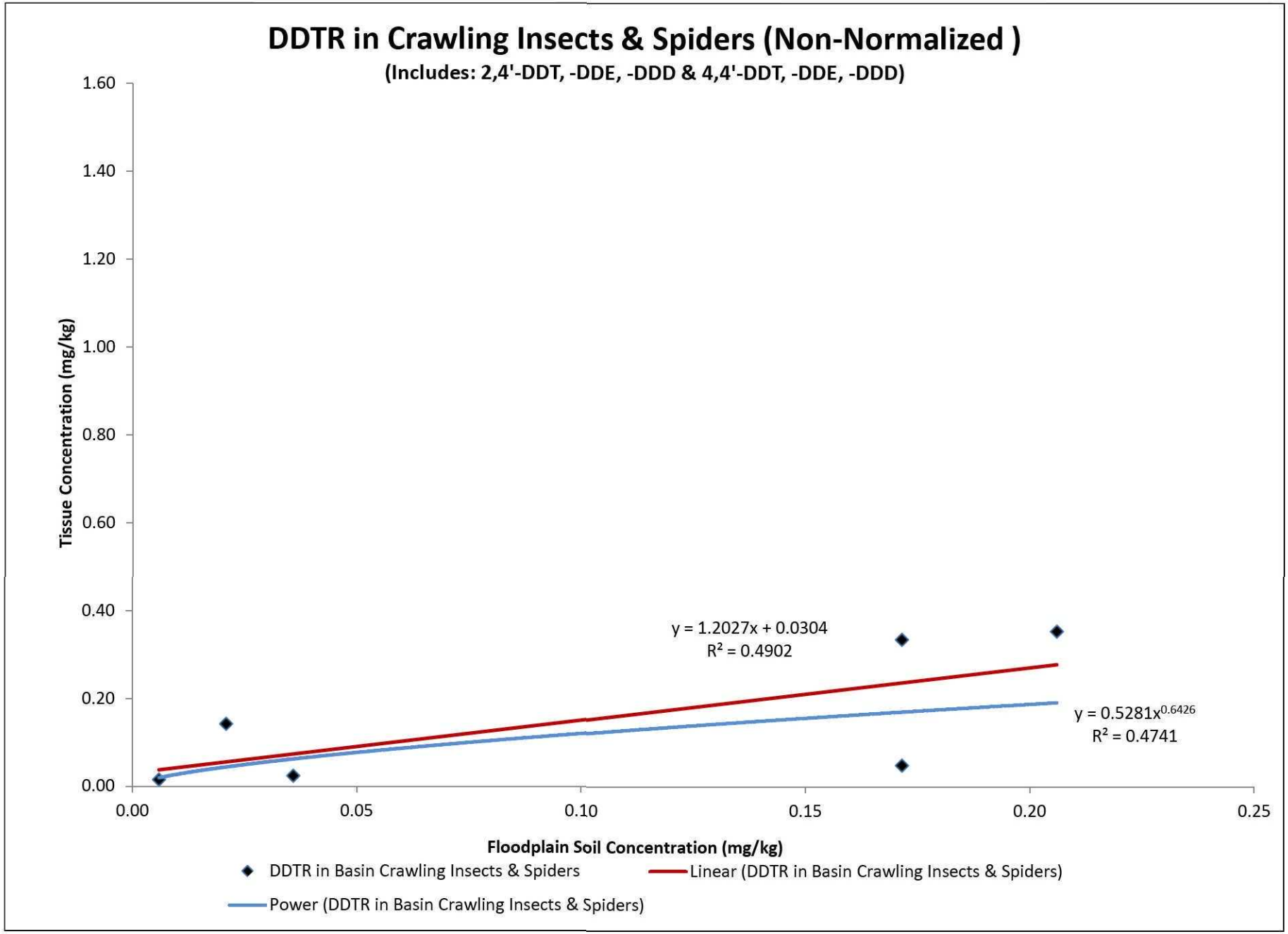
PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-10a



PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

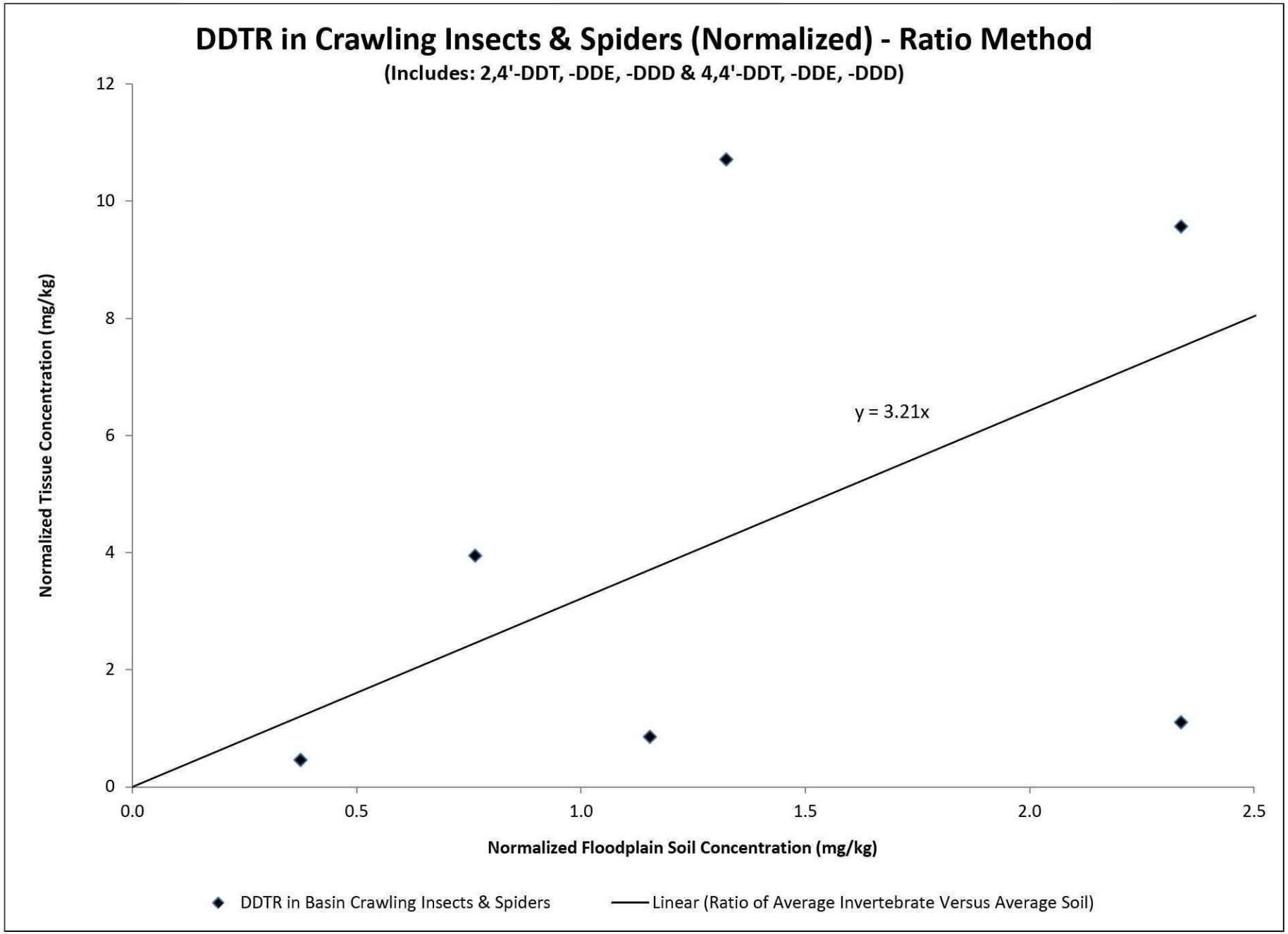
FIGURE D-10b



PREPARED BY/DATE: MKB 01/23/12

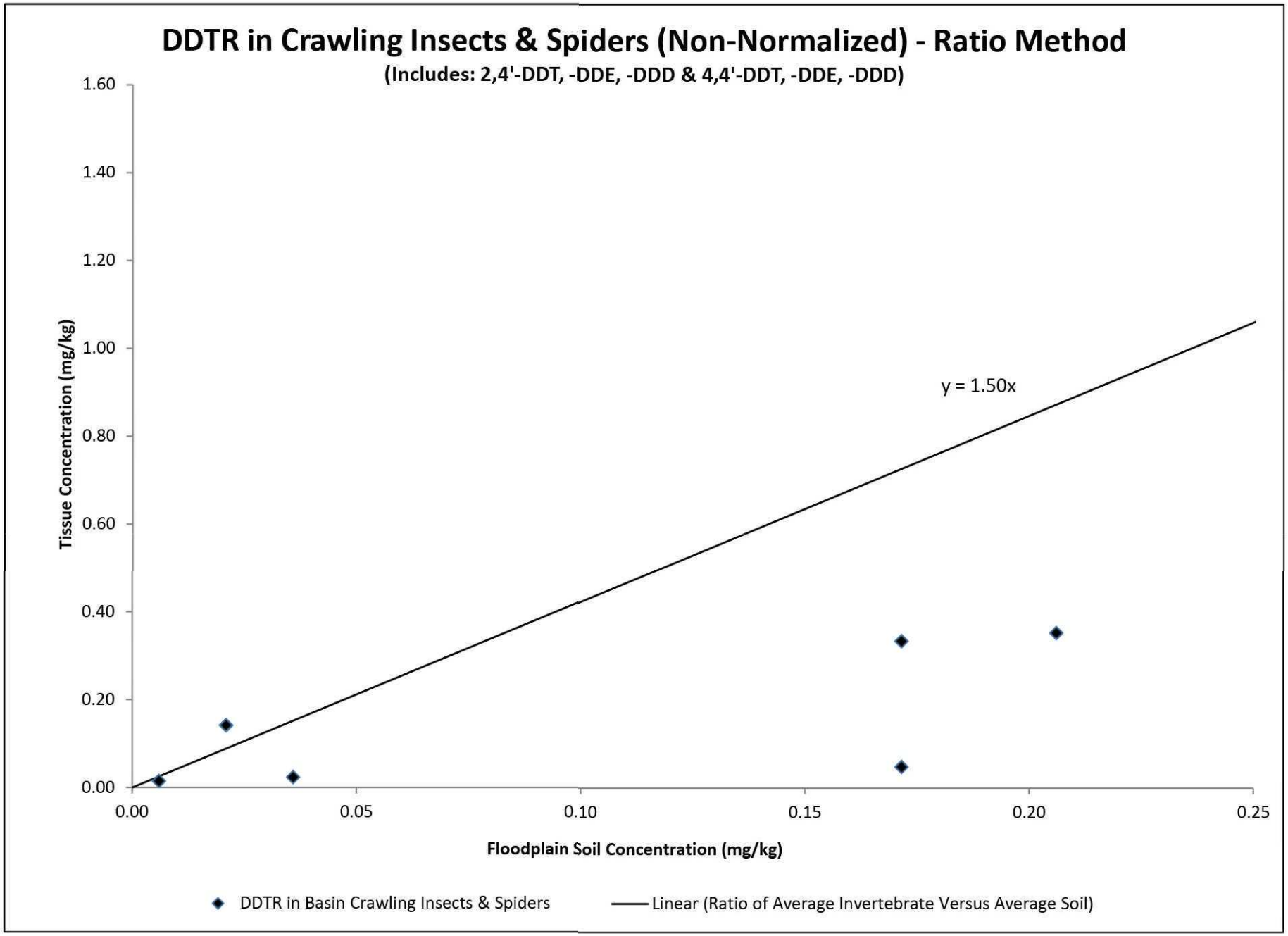
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-10c



PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

FIGURE D-10d



PREPARED BY/DATE: MKB 01/23/12
CHECKED BY/DATE: NSR 1/24/12

APPENDIX D-2

Terrestrial Data Pairings and Regression Statistics – Invertebrate Tissue and Surface Soil

Statistical Analysis of Mercury in Floodplain Soils and Invertebrates

APPENDIX D-2
Statistical Analysis of Mercury in Floodplain Soil and Invertebrates
All Invertebrate Data - 1994 Historical Sample Included
OLIN McINTOSH OU-2

	Avg. Hg Soil Conc. (mg/kg)	Log Avg. Hg Soil Conc. (mg/kg)	Avg. MeHg Inv. Conc. (mg/kg)	Log Avg. MeHg Inv. Conc. (mg/kg)
Flying Insect	0.160	-0.796	0.150	-0.823
Crawling Insect	0.918	-0.037	0.174	-0.760
Flying Insect	0.457	-0.340	0.146	-0.837
Flying Insect	1.000	0.000	0.122	-0.913
Crawling Insect	1.000	0.000	0.004	-2.453
Flying Insect	2.450	0.389	0.066	-1.182
Crawling Insect	2.450	0.389	0.031	-1.502
Spider	1.675	0.224	0.071	-1.152
Flying Insect	1.675	0.224	0.334	-0.477
Crawling Insect	1.675	0.224	0.012	-1.913
Spider-NE	0.561	-0.251	0.080	-1.097
Crawling Insect-NE	0.561	-0.251	0.035	-1.453
Spider-SE	1.290	0.111	0.061	-1.214
Insects - composite 1994 SW	3.783	0.578	0.066	-1.182

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.176257245
R Square	0.031066616
Adjusted R Square	-0.049677832
Standard Error	0.088068071
Observations	14

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.002984134	0.002984134	0.384752351	0.546670216
Residual	12	0.093071821	0.007755985		
Total	13	0.096055955			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.118218203	0.042142893	2.80517534	0.015890985	0.026396728	0.21004	0.026396728	0.210039678
X Variable 1	-0.015444524	0.024899114	-0.62028409	0.546670216	-0.069695032	0.038806	-0.06969503	0.038805984

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.206851142
R Square	0.042787395
Adjusted R Square	-0.036980322
Standard Error	0.514522712
Observations	14

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.142003087	0.142003087	0.536399895	0.477990356
Residual	12	3.176803456	0.264733621		
Total	13	3.318806543			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-1.20143472	0.138147265	-8.69676807	1.58322E-06	-1.502431752	-0.90044	-1.50243175	-0.900437688
X Variable 1	-0.292442542	0.399297147	-0.73239327	0.477990356	-1.162436289	0.577551	-1.16243629	0.577551205

APPENDIX D-2
Statistical Analysis of Mercury in Floodplain Soil and Invertebrates
All Invertebrate Data - 1994 Historical Sample Exccluded
OLIN McINTOSH OU-2

	Avg. Hg Soil Conc. (mg/kg)	Log Avg. Hg Soil Conc. (mg/kg)	Avg. MeHg Inv. Conc. (mg/kg)	Log Avg. MeHg Inv. Conc. (mg/kg)
Flying Insect	0.160	-0.796	0.150	-0.823
Crawling Insect	0.918	-0.037	0.174	-0.760
Flying Insect	0.457	-0.340	0.146	-0.837
Flying Insect	1.000	0.000	0.122	-0.913
Crawling Insect	1.000	0.000	0.004	-2.453
Flying Insect	2.450	0.389	0.066	-1.182
Crawling Insect	2.450	0.389	0.031	-1.502
Spider	1.675	0.224	0.071	-1.152
Flying Insect	1.675	0.224	0.334	-0.477
Crawling Insect	1.675	0.224	0.012	-1.913
Spider-NE	0.561	-0.251	0.080	-1.097
Crawling Insect-NE	0.561	-0.251	0.035	-1.453
Spider-SE	1.290	0.111	0.061	-1.214

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.146610424
R Square	0.021494616
Adjusted R Square	-0.067460418
Standard Error	0.091946553
Observations	13

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.00204282	0.00204282	0.241634624	0.632689387
Residual	11	0.092995854	0.008454169		
Total	12	0.095038674			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.120689082	0.051140301	2.359960337	0.03781652	0.008130039	0.233248	0.008130039	0.233248126
X Variable 1	-0.017847158	0.036306927	-0.49156345	0.632689387	-0.097758166	0.062064	-0.09775817	0.062063849

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.238380099
R Square	0.056825072
Adjusted R Square	-0.028918104
Standard Error	0.533371778
Observations	13

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.188538695	0.188538695	0.662735799	0.43286583
Residual	11	3.129339995	0.284485454		
Total	12	3.317878689			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-1.216669807	0.147985745	-8.2215338	5.03335E-06	-1.542384236	-0.89096	-1.54238424	-0.890955377
X Variable 1	-0.374980997	0.460616027	-0.81408587	0.43286583	-1.388790036	0.638828	-1.38879004	0.638828041

APPENDIX D-2
Statistical Analysis of Mercury in Floodplain Soil and Invertebrates
Spiders
OLIN McINTOSH OU-2

	Avg. Hg Soil Conc. (mg/kg)	Log Avg. Hg Soil Conc. (mg/kg)	Avg. MeHg Inv. Conc. (mg/kg)	Log Avg. MeHg Inv. Conc. (mg/kg)
Spider	1.675	0.224	0.071	-1.152
Spider-NE	0.561	-0.251	0.080	-1.097
Spider-SE	1.290	0.111	0.061	-1.214

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.644195735
R Square	0.414988145
Adjusted R Square	-0.170023711
Standard Error	0.010167758
Observations	3

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	7.33367E-05	7.33367E-05	0.709367068	0.554384433
Residual	1	0.000103383	0.000103383		
Total	2	0.00017672			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	0.083081919	0.016050682	5.176223617	0.12149251	-0.120861332	0.287025	-0.12086	0.28702517
X Variable 1	-0.010704474	0.012709539	-0.84223932	0.554384433	-0.172194479	0.150786	-0.17219	0.15078553

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.701794922
R Square	0.492516112
Adjusted R Square	-0.014967775
Standard Error	0.058730838
Observations	3

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.003347577	0.003347577	0.970505911	0.504764569
Residual	1	0.003449311	0.003449311		
Total	2	0.006796888			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	-1.149805694	0.034228524	-33.5920321	0.018945916	-1.584720334	-0.71489	-1.58472	-0.7148911
X Variable 1	-0.164951102	0.16743881	-0.98514258	0.504764569	-2.292462907	1.962561	-2.29246	1.9625607

APPENDIX D-2
Statistical Analysis of Mercury in Floodplain Soil and Invertebrates
Flying Insects
OLIN McINTOSH OU-2

	Avg. Hg Soil Conc. (mg/kg)	Log Avg. Hg Soil Conc. (mg/kg)	Avg. MeHg Inv. Conc. (mg/kg)	Log Avg. MeHg Inv. Conc. (mg/kg)
Flying Insect	0.160	-0.796	0.150	-0.823
Flying Insect	0.457	-0.340	0.146	-0.837
Flying Insect	1.000	0.000	0.122	-0.913
Flying Insect	2.450	0.389	0.066	-1.182
Flying Insect	1.675	0.224	0.334	-0.477

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.01644507
R Square	0.00027044
Adjusted R Square	-0.33297275
Standard Error	0.11647094
Observations	5

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.10089E-05	1.1009E-05	0.000811541	0.979062428
Residual	3	0.040696443	0.01356548		
Total	4	0.040707452			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	0.16561214	0.088895148	1.86300542	0.159354251	-0.117291892	0.448516	-0.117292	0.44851618
X Variable 1	-0.00178685	0.062724029	-0.0284876	0.979062428	-0.201402709	0.197829	-0.201403	0.197829

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.14606114
R Square	0.02133386
Adjusted R Square	-0.30488819
Standard Error	0.28801207
Observations	5

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.005424722	0.00542472	0.065396738	0.814692553
Residual	3	0.248852863	0.08295095		
Total	4	0.254277585			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	-0.8542589	0.132669344	-6.4390075	0.007595103	-1.276471963	-0.43205	-1.276472	-0.43204583
X Variable 1	-0.07781399	0.304284351	-0.2557279	0.814692553	-1.046182596	0.890555	-1.046183	0.89055462

APPENDIX D-2
Statistical Analysis of Mercury in Floodplain Soil and Invertebrates
Crawling Insects
OLIN McINTOSH OU-2

	Avg. Hg Soil Conc. (mg/kg)	Log Avg. Hg Soil Conc. (mg/kg)	Avg. MeHg Inv. Conc. (mg/kg)	Log Avg. MeHg Inv. Conc. (mg/kg)
Crawling Insect	0.918	-0.037	0.174	-0.760
Crawling Insect	1.000	0.000	0.004	-2.453
Crawling Insect	2.450	0.389	0.031	-1.502
Crawling Insect	1.675	0.224	0.012	-1.913
Crawling Insect-NE	0.561	-0.251	0.035	-1.453

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.278046664
R Square	0.077309948
Adjusted R Square	-0.2302534
Standard Error	0.077424552
Observations	5

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.001506809	0.001506809	0.251362678	0.650595952
Residual	3	0.017983684	0.005994561		
Total	4	0.019490493			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.085507595	0.076553498	1.116965217	0.345406451	-0.158119803	0.329135	-0.1581198	0.32913499
X Variable 1	-0.02591787	0.051695044	-0.501360827	0.650595952	-0.190434571	0.138599	-0.1904346	0.13859883

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.153691619
R Square	0.023621114
Adjusted R Square	-0.30183851
Standard Error	0.712856513
Observations	5

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.036881408	0.036881408	0.072577708	0.805086894
Residual	3	1.524493223	0.508164408		
Total	4	1.561374631			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-1.59081136	0.33225592	-4.787909759	0.017326601	-2.648197991	-0.53342	-2.648198	-0.5334247
X Variable 1	-0.38808772	1.440549814	-0.269402501	0.805086894	-4.972560154	4.196385	-4.9725602	4.19638471

APPENDIX D-2
Statistical Analysis of Mercury in Floodplain Soil and Invertebrates
Crawling Insects and Spider
OLIN McINTOSH OU-2

	Avg. Hg Soil Conc. (mg/kg)	Log Avg. Hg Soil Conc. (mg/kg)	Avg. MeHg Inv. Conc. (mg/kg)	Log Avg. MeHg Inv. Conc. (mg/kg)
Crawling Insect	0.918	-0.037	0.174	-0.760
Crawling Insect	1.000	0.000	0.004	-2.453
Crawling Insect	2.450	0.389	0.031	-1.502
Spider	1.675	0.224	0.071	-1.152
Crawling Insect	1.675	0.224	0.012	-1.913
Spider-NE	0.561	-0.251	0.080	-1.097
Crawling Insect-NE	0.561	-0.251	0.035	-1.453
Spider-SE	1.290	0.111	0.061	-1.214

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.287885394
R Square	0.082878
Adjusted R Square	-0.069975667
Standard Error	0.055786301
Observations	8

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.0016874	0.001687402	0.542204855	0.489297562
Residual	6	0.01867267	0.003112111		
Total	7	0.02036007			

	Coefficients	*Standard Erro*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.08891012	0.04578438	1.941931135	0.100173335	-0.02312023	0.20094	-0.0231202	0.20094047
X Variable 1	-0.024027637	0.03263092	-0.736345608	0.489297562	-0.10387263	0.055817	-0.1038726	0.05581736

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.172658069
R Square	0.029810809
Adjusted R Square	-0.13188739
Standard Error	0.564071751
Observations	8

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.05865935	0.058659354	0.184360798	0.682642427
Residual	6	1.90906164	0.31817694		
Total	7	1.96772099			

	Coefficients	*Standard Erro*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-1.422598255	0.20496873	-6.940562526	0.00044352	-1.92413866	-0.92106	-1.9241387	-0.9210579
X Variable 1	-0.39790754	0.9267186	-0.429372563	0.682642427	-2.66550626	1.869691	-2.6655063	1.86969118

Statistical Analysis of DDTR (Normalized) in Floodplain Soils and Invertebrates

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
All Invertebrate Data (Normalized) - 1994 Historical Sample Included
OLIN McINTOSH OU-2

	Norm. Soil Conc. (mg/kg)	Log Norm. Soil Conc. (mg/kg)	Norm. Tissue Conc. (mg/kg)	Log Norm. Tissue Conc. (mg/kg)
Flying Insect	3.619	0.559	20.609	1.314
Crawling Insect	1.324	0.122	10.714	1.030
Flying Insect	2.585	0.413	8.431	0.926
Flying Insect	1.153	0.062	6.880	0.838
Crawling Insect	1.153	0.062	0.855	-0.068
Flying Insect	0.375	-0.426	3.008	0.478
Crawling Insect	0.375	-0.426	0.461	-0.337
Spider-NE	2.337	0.369	9.569	0.981
Crawling Insect-NE	2.337	0.369	1.105	0.043
Spider-SE	0.764	-0.117	3.949	0.596
Insects-SW (Composite, 1994)	31.124	1.493	3.439	0.536

SUMMARY OUTPUT - LINEAR REGRESSION (NORMALIZED)

Regression Statistics	
Multiple R	0.074985
R Square	0.005623
Adjusted R Square	-0.104864
Standard Error	6.263334
Observations	11

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.996432	1.9964316	0.0508913	0.826559004
Residual	9	353.0642	39.229355		
Total	10	355.0606			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	6.488126	2.112868	3.0707675	0.0133374	1.708486768	11.26777	1.70848677	11.2677652
X Variable 1	-0.049875	0.221085	-0.225591	0.826559	-0.55000378	0.450254	-0.5500038	0.45025424

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.332602
R Square	0.110624
Adjusted R Square	0.011805
Standard Error	0.511586
Observations	11

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.292985	0.2929846	1.1194571	0.317605643
Residual	9	2.355482	0.2617203		
Total	10	2.648467			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.503634	0.168806	2.9834996	0.0153621	0.121767202	0.8855	0.1217672	0.8855003
X Variable 1	0.322073	0.304404	1.058044	0.3176056	-0.36653683	1.010682	-0.3665368	1.01068242

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
All Invertebrate Data (Normalized) - 1994 Historical Sample Excluded
OLIN McINTOSH OU-2

	Norm. Soil Conc. (mg/kg)	Log Norm. Soil Conc. (mg/kg)	Norm. Tissue Conc. (mg/kg)	Log Norm. Tissue Conc. (mg/kg)
Flying Insect	3.619	0.559	20.609	1.314
Crawling Insect	1.324	0.122	10.714	1.030
Flying Insect	2.585	0.413	8.431	0.926
Flying Insect	1.153	0.062	6.880	0.838
Crawling Insect	1.153	0.062	0.855	-0.068
Flying Insect	0.375	-0.426	3.008	0.478
Crawling Insect	0.375	-0.426	0.461	-0.337
Spider-NE	2.337	0.369	9.569	0.981
Crawling Insect-NE	2.337	0.369	1.105	0.043
Spider-SE	0.764	-0.117	3.949	0.596

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.730912
R Square	0.534232
Adjusted R Square	0.476011
Standard Error	4.489675
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	184.9609	184.9609	9.17593	0.01632978
Residual	8	161.2575	20.15718		
Total	9	346.2184			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-0.22848	2.65232	-0.08614	0.933469	-6.34474188	5.887778	-6.3447419	5.8877776
X Variable 1	4.235421	1.398207	3.02918	0.01633	1.01114955	7.459693	1.01114955	7.45969339

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.577171
R Square	0.333127
Adjusted R Square	0.249767
Standard Error	0.469712
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.881696	0.881696	3.996281	0.08063233
Residual	8	1.765034	0.220629		
Total	9	2.64673			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.490175	0.155207	3.158195	0.013431	0.13226638	0.848084	0.13226638	0.84808449
X Variable 1	0.913575	0.457	1.99907	0.080632	-0.14026895	1.967419	-0.140269	1.96741941

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
Flying Insects (Normalized)
OLIN McINTOSH OU-2

	Norm. Soil Conc. (mg/kg)	Log Norm. Soil Conc. (mg/kg)	Norm. Tissue Conc. (mg/kg)	Log Norm. Tissue Conc. (mg/kg)
Flying Insect	3.619	0.559	20.609	1.314
Flying Insect	2.585	0.413	8.431	0.926
Flying Insect	1.153	0.062	6.880	0.838
Flying Insect	0.375	-0.426	3.008	0.478

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.913274
R Square	0.834069
Adjusted R Square	0.751103
Standard Error	3.792309
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	144.581	144.581043	10.0531927	0.086726295
Residual	2	28.76321	14.3816047		
Total	3	173.3443			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.474005	3.481503	0.13614948	0.90417084	-14.5056931	15.4537	-14.5056931	15.45370269
X Variable 1	4.788884	1.510366	3.17067701	0.08672629	-1.70969805	11.28747	-1.70969805	11.2874659

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.941322
R Square	0.886087
Adjusted R Square	0.829131
Standard Error	0.141873
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.313134	0.31313376	15.5572614	0.058678047
Residual	2	0.040256	0.02012782		
Total	3	0.353389			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.777019	0.076401	10.1702455	0.00953003	0.448291289	1.105747	0.44829129	1.105747184
X Variable 1	0.737592	0.187003	3.94426944	0.05867805	-0.0670189	1.542203	-0.0670189	1.542202756

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
Crawling Insects (Normalized)
OLIN McINTOSH OU-2

	Norm. Soil Conc. (mg/kg)	Log Norm. Soil Conc. (mg/kg)	Norm. Tissue Conc. (mg/kg)	Log Norm. Tissue Conc. (mg/kg)
Crawling Insect	1.324	0.122	10.714	1.030
Crawling Insect	1.153	0.062	0.855	-0.068
Crawling Insect	0.375	-0.426	0.461	-0.337
Crawling Insect-NE	2.337	0.369	1.105	0.043

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.07352
R Square	0.005405
Adjusted R Square	-0.49189
Standard Error	6.058893
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.399004	0.399004	0.010869	0.92648035
Residual	2	73.42037	36.71019		
Total	3	73.81938			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.697272	6.387494	0.422274	0.713889	-24.7858966	30.18044	-24.7858966	30.18044
X Variable 1	0.45194	4.334963	0.104255	0.92648	-18.1998991	19.10378	-18.1998991	19.103779

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.435448
R Square	0.189615
Adjusted R Square	-0.21558
Standard Error	0.65809
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.202666	0.202666	0.467963	0.564551697
Residual	2	0.866164	0.433082		
Total	3	1.06883			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.142499	0.331012	0.430495	0.708787	-1.28173036	1.566729	-1.28173036	1.5667286
X Variable 1	0.781067	1.141779	0.684079	0.564552	-4.13161236	5.693745	-4.13161236	5.6937455

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
Crawling Insects & Spiders (Normalized)
OLIN McINTOSH OU-2

	Norm. Soil Conc. (mg/kg)	Log Norm. Soil Conc. (mg/kg)	Norm. Tissue Conc. (mg/kg)	Log Norm. Tissue Conc. (mg/kg)
Crawling Insect	1.324	0.122	10.714	1.030
Crawling Insect	1.153	0.062	0.855	-0.068
Crawling Insect	0.375	-0.426	0.461	-0.337
Spider-NE	2.337	0.369	9.569	0.981
Crawling Insect-NE	2.337	0.369	1.105	0.043
Spider-SE	0.764	-0.117	3.949	0.596

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.348032
R Square	0.121126
Adjusted R Square	-0.09859
Standard Error	4.819442
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	12.80459	12.80459	0.55128	0.499029756
Residual	4	92.9081	23.22703		
Total	5	105.7127			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	1.71039	4.171964	0.409972	0.702833	-9.872838068	13.29362	-9.8728381	13.2936174
X Variable 1	1.97694	2.662609	0.742482	0.49903	-5.415647511	9.369527	-5.4156475	9.369527403

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.492504
R Square	0.24256
Adjusted R Square	0.0532
Standard Error	0.560274
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.402097	0.402097	1.280945	0.320975452
Residual	4	1.255626	0.313907		
Total	5	1.657723			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.315526	0.234555	1.345213	0.249759	-0.335701971	0.966754	-0.335702	0.966754014
X Variable 1	0.932979	0.824341	1.131788	0.320975	-1.355758106	3.221717	-1.3557581	3.22171692

Statistical Analysis of DDTR (Non-Normalized) in Floodplain Soils and Invertebrates

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
All Invertebrate Data (Non-Normalized) - 1994 Historical Sample Included
OLIN McINTOSH OU-2

	Soil Conc. (mg/kg)	Log Soil Conc. (mg/kg)	Tissue Conc. (mg/kg)	Log Tissue Conc. (mg/kg)
Flying Insect	0.216	-0.666	0.659	-0.181
Crawling Insect	0.206	-0.686	0.354	-0.452
Flying Insect	0.134	-0.874	0.337	-0.472
Flying Insect	0.036	-1.445	0.282	-0.550
Crawling Insect	0.036	-1.445	0.024	-1.621
Flying Insect	0.006	-2.225	0.120	-0.920
Crawling Insect	0.006	-2.225	0.015	-1.818
Spider-NE	0.172	-0.766	0.335	-0.475
Crawling Insect-NE	0.172	-0.766	0.049	-1.313
Spider-SE	0.021	-1.680	0.142	-0.847
Insects-SW (Composite, 1994)	1.432	0.156	0.130	-0.886

SUMMARY OUTPUT - LINEAR ANALYSIS

Regression Statistics	
Multiple R	0.01873
R Square	0.000351
Adjusted R Square	-0.11072
Standard Error	0.204242
Observations	11

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.000132	0.000132	0.003158	0.956411069
Residual	9	0.375432	0.041715		
Total	10	0.375564			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.224457	0.070775	3.171425	0.01134	0.064353172	0.38456	0.06435317	0.38456033
X Variable 1	-0.00886	0.157596	-0.0562	0.956411	-0.36536314	0.34765	-0.36536314	0.34764966

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.469806
R Square	0.220718
Adjusted R Square	0.134131
Standard Error	0.486129
Observations	11

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.602405	0.602405	2.549094	0.144821954
Residual	9	2.12689	0.236321		
Total	10	2.729295			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-0.47962	0.283337	-1.69275	0.124753	-1.12057161	0.161334	-1.12057161	0.16133416
X Variable 1	0.337416	0.211336	1.596588	0.144822	-0.14065858	0.815491	-0.14065858	0.81549121

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
All Invertebrate Data (Non-Normalized) - 1994 Historical Sample Excluded
OLIN McINTOSH OU-2

	Soil Concentration (mg/kg)	Log Soil Conc. (mg/kg)	Tissue Conc. (mg/kg)	Log Tissue Conc. (mg/kg)
Flying Insect	0.216	-0.666	0.659	-0.181
Crawling Insect	0.206	-0.686	0.354	-0.452
Flying Insect	0.134	-0.874	0.337	-0.472
Flying Insect	0.036	-1.445	0.282	-0.550
Crawling Insect	0.036	-1.445	0.024	-1.621
Flying Insect	0.006	-2.225	0.120	-0.920
Crawling Insect	0.006	-2.225	0.015	-1.818
Spider-NE	0.172	-0.766	0.335	-0.475
Crawling Insect-NE	0.172	-0.766	0.049	-1.313
Spider-SE	0.021	-1.680	0.142	-0.847

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.685337
R Square	0.469686
Adjusted R Square	0.403397
Standard Error	0.155795
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.171977	0.171977	7.085414	0.02872321
Residual	8	0.194176	0.024272		
Total	9	0.366153			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.072414	0.077525	0.934077	0.377596	-0.10635869	0.251187	-0.10635869	0.25118742
X Variable 1	1.588386	0.596724	2.661844	0.028723	0.212338204	2.964433	0.2123382	2.96443327

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.593202
R Square	0.351888
Adjusted R Square	0.270874
Standard Error	0.470189
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.960263	0.960263	4.34355	0.070661303
Residual	8	1.768623	0.221078		
Total	9	2.728885			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-0.1881	0.35713	-0.5267	0.612688	-1.01164542	0.635443	-1.01164542	0.63544296
X Variable 1	0.529651	0.254137	2.084119	0.070661	-0.05638923	1.115691	-0.05638923	1.11569089

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
Flying Insects (Non-Normalized)
OLIN McINTOSH OU-2

	Soil Concentration (mg/kg)	Log Soil Conc. (mg/kg)	Tissue Conc. (mg/kg)	Log Tissue Conc. (mg/kg)
Flying Insect	0.216	-0.666	0.659	-0.181
Flying Insect	0.134	-0.874	0.337	-0.472
Flying Insect	0.036	-1.445	0.282	-0.550
Flying Insect	0.006	-2.225	0.120	-0.920

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.945132
R Square	0.893275
Adjusted R Sc	0.839913
Standard Erro	0.090448
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.136947	0.136947	16.73982	0.054867514
Residual	2	0.016362	0.008181		
Total	3	0.153309			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.131333	0.06997	1.876989	0.201324	-0.16972362	0.432389	-0.1697236	0.432389448
X Variable 1	2.233033	0.545783	4.091433	0.054868	-0.11528	4.581346	-0.11528	4.581345863

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.957161
R Square	0.916156
Adjusted R Sc	0.874235
Standard Erro	0.107866
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.254273	0.254273	21.85392	0.042839442
Residual	2	0.02327	0.011635		
Total	3	0.277543			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.013041	0.128179	0.101743	0.928242	-0.53846663	0.564549	-0.5384666	0.564549225
X Variable 1	0.417355	0.089277	4.674818	0.042839	0.033225849	0.801484	0.03322585	0.801483847

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
Crawling Insects (Non-Normalized)
OLIN McINTOSH OU-2

	Soil Concentration (mg/kg)	Log Soil Conc. (mg/kg)	Tissue Conc. (mg/kg)	Log Tissue Conc. (mg/kg)
Crawling Insect	0.206	-0.686	0.354	-0.452
Crawling Insect	0.036	-1.445	0.024	-1.621
Crawling Insect	0.006	-2.225	0.015	-1.818
Crawling Insect-NE	0.172	-0.766	0.049	-1.313

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.744158
R Square	0.553771
Adjusted R Square	0.330657
Standard Error	0.133164
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.044013	0.044013	2.482007	0.255841886
Residual	2	0.035465	0.017733		
Total	3	0.079478			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-0.01835	0.105376	-0.17414	0.877789	-0.471745321	0.435046	-0.4717453	0.4350456
X Variable 1	1.227287	0.779013	1.575439	0.255842	-2.124534302	4.579107	-2.1245343	4.5791074

SUMMARY OUTPUT - REGRESSION ANALYSIS

Regression Statistics	
Multiple R	0.802635
R Square	0.644223
Adjusted R Square	0.466334
Standard Error	0.440617
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.703088	0.703088	3.621491	0.197365263
Residual	2	0.388287	0.194143		
Total	3	1.091375			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-0.43496	0.505581	-0.86032	0.480277	-2.610297314	1.740378	-2.6102973	1.7403779
X Variable 1	0.676313	0.355389	1.903022	0.197365	-0.852802159	2.205428	-0.8528022	2.2054275

APPENDIX D-2
Statistical Analysis of DDTR in Floodplain Soil and Invertebrates
Crawling Insects & Spiders (Non-Normalized)
OLIN McINTOSH OU-2

	Soil Concentration (mg/kg)	Log Soil Conc. (mg/kg)	Tissue Conc. (mg/kg)	Log Tissue Conc. (mg/kg)
Crawling Insect	0.206	-0.686	0.354	-0.452
Crawling Insect	0.036	-1.445	0.024	-1.621
Crawling Insect	0.006	-2.225	0.015	-1.818
Spider-NE	0.172	-0.766	0.335	-0.475
Crawling Insect-NE	0.172	-0.766	0.049	-1.313
Spider-SE	0.021	-1.680	0.142	-0.847

SUMMARY OUTPUT - LINEAR REGRESSION

Regression Statistics	
Multiple R	0.70016
R Square	0.490224
Adjusted R Square	0.36278
Standard Error	0.123649
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.058811	0.058811	3.846578	0.121377826
Residual	4	0.061157	0.015289		
Total	5	0.119968			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.030424	0.080361	0.378589	0.72423	-0.192695126	0.253543	-0.1926951	0.25354296
X Variable 1	1.202676	0.613213	1.96127	0.121378	-0.499876421	2.905229	-0.4998764	2.90522937

SUMMARY OUTPUT - POWER REGRESSION

Regression Statistics	
Multiple R	0.688561
R Square	0.474116
Adjusted R Square	0.342645
Standard Error	0.473644
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.80902	0.80902	3.606246	0.130387402
Residual	4	0.897354	0.224338		
Total	5	1.706374			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-0.27725	0.46853	-0.59174	0.585852	-1.578094884	1.023602	-1.5780949	1.02360231
X Variable 1	0.642607	0.33839	1.899012	0.130387	-0.296914833	1.582129	-0.2969148	1.58212877

APPENDIX E

Determination of Target Invertebrate Tissue Concentration by Back Calculation of Risk Equations

TABLE E-1

CALCULATION OF TARGET INVERTERBATE CONCENTRATION - METHYLMERCURY
Remedial Goal Option Report for Floodplain Surface Soil
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_I	C_I	P_S	EDD [(b)] (mg/kg-day)	NOAEL/LOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Terrestrial Receptors													
Carolina Wren	Methylmercury	2.74E-06	0.0051	0.0200	0.814	0.0043	1.00	1.00	**0.076**	0.10	6.22E-02	0.060	**1.0**

Notes:
(a) Site-specific BAF calculated using 6 data pairs of insect and soil samples from 2010.
(b) EDD (mg/kg·day) = NFIR x AUF x $[(C_I \times P_I) + (C_S \times P_S)]$ + $(IR_W \times C_W)/BW$

The C_I dietary component consists of all insects for the Carolina Wren.

Green highlighted entries represent target concentrations in controlling media needed to achieve the target HQ=1.

REVISED BY/DATE: MKB 4/20/11

CHECKED BY/DATE: NSR 4/25/11

TABLE E-2

NOAEL RISK CALCULATIONS - DDTR
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_I	C_I	P_S	EDD [(a)] (mg/kg-day)	NOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Terrestrial Receptors														
Carolina Wren	DDTR	1.35E-04	0.10	1.57	0.0200	0.814	0.00430	1.00	1.00	**0.280**	0.10	2.36E-01	0.227	**1.0**

Notes:

REVISED BY/DATE: MKB 4/26/11
CHECKED BY/DATE: NSR 4/28/11

(a) EDD (mg/kg·day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)]
+ (IRW x CW)/BW
The C_I dietary component consists of all insects.

Green highlighted entries represent target concentrations in controlling media needed to achieve the target HQ=1.

TABLE E-3

LOAEL RISK CALCULATIONS - DDTR
Updated Ecological Risk Assessment
Olin - McIntosh
Operable Unit 2
McIntosh, Alabama

Receptor	Analyte	EPC in Water, C_W (mg/L) (a)	EPC in Soil, C_S (mg/kg) (b)	EPC in Sediment, C_{SED} (mg/kg) (b)	Body Weight (BW) (kg)	BW Normalized Food Ingestion Rate (IR_F) (kg/day)	Water Ingestion Rate (IR_W) (L/day)	AUF	P_I	C_I	P_S	EDD [(a)] (mg/kg-day)	LOAEL TRV (mg/kg-day)	Hazard Quotient (HQ)
Terrestrial Receptors														
Carolina Wren	DDTR	1.35E-04	0.12	1.57	0.020	0.814	0.00430	1.00	1.00	**0.35**	0.10	2.95E-01	0.281	**1.0**

Notes:

REVISED BY/DATE: MKB 4/26/11
CHECKED BY/DATE: NSR 4/28/11

(a) EDD (mg/kg·day) = NFIR x AUF x Σ[(Ci x Pi) + (CS/SED x PS)]
+ (IRW x CW)/BW
The C_I dietary component consists of all insects.
Green highlighted entries represent target concentrations in controlling media needed to achieve the target HQ=1.