

## Appendix B

# Description of Evaluation Parameters Used in the NSI Data Evaluation

Chapter 2 of this document presented an overview of the methodology used in the evaluation of the NSI data. This appendix describes in greater detail the screening values and other parameters used in the NSI data evaluation. The actual parameter values used are presented in Appendix C. For the purpose of discussion, the sediment evaluation parameters have been placed into two groups: (1) those used to assess potential impacts on aquatic life, and (2) those used to assess potential impacts on human health.

### *Aquatic Life Assessments*

To evaluate the potential threat to aquatic life from chemical contaminants detected in sediments, measured concentrations of contaminants were compared to sediment chemistry screening levels. The results of toxicity tests to indicate the actual toxicity of sediment samples to species of aquatic organisms were also evaluated for the *National Sediment Quality Survey*.

Sediment chemistry screening levels are reference values that provide evidence of sediment contaminant concentrations that could pose a significant threat to aquatic life based on statistical significance. Although the quantitative relationship between statistical significance and expected ecological effects is not fully understood, we presume that these values are related to expected ecological effects as is the presumption of other EPA assessment approaches (USEPA, 1985). Several different approaches, based on causal or empirical/statistical correlative methodologies, have been developed for deriving screening levels of sediment contaminants. Each of these approaches attempts to predict contaminant concentration levels to provide protection for benthic species, which are extrapolated to represent the entire aquatic community for this evaluation. For the purpose of this analysis, the screening tools selected include the following:

- EPA's draft equilibrium partitioning sediment guidelines (ESGs) for nonionic organics using an equilibrium partitioning approach (USEPA, 1992a, 2000a).
- EPA's draft equilibrium partitioning sediment guidelines (ESGs) for mixtures of polycyclic aromatic hydrocarbons (PAHs) using an equilibrium partitioning approach (USEPA, 1992a, 2000b).
- The sum of simultaneously extracted divalent transition metals concentrations minus the acid-volatile sulfide concentration ([SEM]-[AVS]), also based on an equilibrium partitioning approach (USEPA, 2000c).
- Logistic regression model (Field et al., 1999, 2001 [in press]).

The principles behind the development of each of these sediment chemistry screening values are discussed below. The sediment toxicity tests are also briefly described in this section.

### *Equilibrium Partitioning Approaches*

The potential toxicity of sediment-associated nonionic organic chemicals and divalent metals is indicated by the amount of the contaminant that is uncomplexed or freely available in the interstitial (pore) water. The bioavailability and toxicity of nonionic organic chemicals and divalent metals in sediments are mediated by several physical, chemical, and biological factors, including sediment grain size, particulate and dissolved organic carbon, and sulfide produced by sulfate-reducing bacteria (Di Toro et al., 1991, 1992; Howard and Evans, 1993, USEPA, 2000a). For nonionic organic chemicals, sorption

to the organic carbon dissolved in the interstitial water and bound to sediment particles is the most important factor affecting bioavailability. Sulfide, specifically the reactive solid-phase sulfide fraction that can be extracted by cold hydrochloric acid (acid-volatile sulfide, or AVS), appears to control the bioavailability of most divalent metal ions because of the sulfide ions' high affinity for divalent metals, resulting in the formation of insoluble metal sulfides in anaerobic sediments (USEPA, 2000c).

When the concentrations of nonionic organic chemicals and divalent metals were measured in pore water extracted from spiked sediment and field-collected sediment used in toxicity tests, the biological effects observed in those tests occurred at similar pore water concentrations, even when different types of sediments were used, typically within a factor of 2 (Di Toro et al., 1991, 1992). Biological effects also occurred at similar concentrations in tests with different sediment types containing different amounts of organic carbon (OC) when (1) the dry-weight sediment concentrations of nonionic organic chemicals were normalized for organic carbon content (i.e.,  $\mu\text{g chemical/g}_{\text{OC}}$ ) and (2) when the difference between molar concentrations of simultaneously extracted metals ([SEM]) in the sediment exceeded the molar concentration of AVS ([AVS]) in the sediments by similar amounts (the mortality of sensitive species increases in the range of 1.5 to 12.5  $\mu\text{mol}$  of SEM per  $\mu\text{mol}$  of AVS). Most importantly, the effects concentrations in the sediment could be predicted from the effects concentrations determined in water-only exposures to these chemicals. Most measurements of sediment chemical concentrations are made from whole sediment samples and converted to units of chemical per dry-weight of sediment, because of the difficulties in extracting the pore water. However, when dry-weight concentrations of nonionic organics and metals were used to plot concentration-response curves of the toxicity of different sediments, biological effects occurred at different dry-weight concentrations when measured in different sediments (Luoma, 1983; USEPA, 2000a). To develop advisory levels for comparing the toxicity of different chemicals in different sediments, it was necessary to examine the role of organic carbon and other complexing factors in the bioavailability of chemicals in sediment.

In sediment, the partitioning of a nonionic organic chemical between organic carbon and pore water and the partitioning of a divalent metal between the solid and solution phases are assumed to be at equilibrium. The fugacity (activity) of the chemical in each of these phases is the same at equilibrium. Fugacity describes mathematically the rates at which chemicals diffuse or are transported between phases (Mackay, 1991). Hence, an organism in the sediment is assumed to receive an equivalent exposure from water only or from any equilibrated phase. The pathway of exposure might include pore water (respiration), sediment carbon (ingestion), sediment organism (ingestion), or a mixture of routes. The biological effect is produced by the chemical activity of the single phase or the equilibrated system (Di Toro et al., 1991). The equilibrium partitioning approach uses this partitioning theory to relate the dry-weight sediment concentration of a particular chemical that causes an adverse biological effect to the equivalent free chemical concentration in pore water and to the concentration sorbed to sediment organic carbon or bound to sulfide.

The processes that govern the partitioning of chemical contaminants among sediments, pore water, and biota are better understood for some kinds of chemicals than for others. Partitioning of nonionic hydrophobic organic compounds between sediments and pore water is highly correlated with the organic carbon content of sediments, but it does not account for all of the toxicity variation observed between sediment and water-only experimental exposures. Other factors that can affect biological responses are not considered in the model. The equilibrium partitioning approach has been tested using only nonionic organic chemicals with octanol/water partition coefficients ( $\log K_{\text{ow,s}}$ ) between 3.8 and 5.3. However, because the theory should be applicable to nonionic organic chemicals with  $\log K_{\text{ow,s}}$  from 2.0 to 5.5 (Dave Hansen, EPA ORD-Narragansett, pers. commun., April 17, 1995), nonionic organic chemicals with  $\log K_{\text{ow,s}}$  in this range were evaluated for the analysis of NSI data. For trace metals, concentrations of sulfides and organic carbon have been identified as important factors that control the phase associations and, therefore, the bioavailability of trace metals in anoxic sediments. However, models that can use these factors to predict the bioavailability of trace metals in sediments are not fully developed (see below). Mechanisms that control the partitioning of nonionic and nonpolar organic compounds with  $\log$

$K_{ow}$ s of less than 2.0 or greater than 5.5 and polar organic compounds in sediments, and affect their toxicity to benthic organisms, are less well understood. Models for predicting biological effects from concentrations of such compounds have not yet been developed; therefore, these chemicals have not been evaluated using equilibrium partitioning approaches.

#### *Draft Sediment Equilibrium Partitioning Sediment Guidelines (ESGs) for Nonionic Organics*

The equilibrium partitioning model was selected for use in this assessment due to its ability to predict sediment contaminant concentrations that are protective for benthic aquatic life from direct toxicity due to that contaminant (or contaminants in the case of metals mixtures and PAH mixtures). The predominant phase for sorption of nonionic organic chemicals to sediment particles appears to be organic carbon for sediments in which the fraction of organic carbon ( $f_{oc}$ ) is greater than 0.2 percent. When the fraction of organic carbon is less than 0.2 percent, other factors, such as particle size and sorption to nonorganic mineral fractions, play a relatively important role (Karickhoff, 1984).

The partitioning of a chemical between the interstitial water and sediment organic carbon is explained by the sediment/pore water partition coefficient for a chemical,  $K_p$ , which is equal to the organic carbon content of the sediment ( $f_{oc}$ ) multiplied by the sediment particle organic carbon partition coefficient ( $K_{oc}$ ).  $K_p$  is the ratio of the concentration of the chemical in the sediment to the concentration of the chemical in the pore water. Normalizing the dry-weight concentration of the chemical in sediment to organic carbon is as appropriate as using the interstitial water concentration of the chemical because organic carbon in the sediment can also bind the chemical and affect its bioavailability and toxicity. The particle organic carbon partition coefficient ( $K_{oc}$ ) is related to the chemical's octanol-water partition coefficient ( $K_{ow}$ ) by the following equation (Di Toro et al., 1991, Di Toro and McGrath, 2000):

$$\log K_{oc} = 0.00028 + 0.983(\log K_{ow})$$

The octanol/water partition coefficient for each chemical can thus predict the likelihood of the chemical to complex or sorb to organic carbon, when measured with modern experimental techniques that provide the most accurate estimate of this parameter. The concentration of the chemical on sediment particles ( $C_s$ ) is then equal to the dissolved concentration of chemical ( $C_d$ ) multiplied by the organic carbon content of the sediment ( $f_{oc}$ ) and the particle organic carbon partition coefficient ( $K_{oc}$ ), when  $f_{oc}$  is greater than 0.2 percent (USEPA, 2000a), thus normalizing the dry-weight sediment concentration of the chemical to the organic carbon content of the sediment:

$$C_s = C_d f_{oc} K_{oc}$$

The value for the dissolved concentration of chemical ( $C_d$ ) is derived from the chronic or acute value in EPA's water quality criteria (USEPA, 1985, GLI, 1995). Freshwater and saltwater acute and chronic values are based on the results of acceptable laboratory tests conducted to determine the toxicity of a chemical in water to a variety of species of aquatic organisms, and they represent levels below which adverse effects are not expected. An evaluation of data from the water quality criteria documents and benthic colonization experiments demonstrated that benthic species have chemical sensitivities similar to those of water column species (Di Toro et al., 1991). Therefore, these guidelines can be used to protect benthic aquatic life from direct toxicity due to the specific contaminant(s).

EPA has developed draft equilibrium partitioning sediment guidelines (ESGs) for the protection of aquatic life for 34 specific nonionic contaminants listed in Table B-1. In the NSI data evaluation, sediment chemistry values exceeding draft ESG guidelines derived from acute values were used to classify stations as Tier 1. Draft ESG guidelines obtained from chronic values were used for Tier 2 classification.

**Table B-1. EPA Aquatic Life Secondary Acute/Chronic Values (SAV/SCV), Final Acute/ Chronic Values (FAV/FCV), Draft Equilibrium Partitioning Sediment Guideline (ESG), Log K<sub>ow</sub>, and Log K<sub>oc</sub> Values.**

CAS Number	Chemical Name	Log K <sub>ow</sub>	SAV (µg/L)	SCV (µg/L)	Log K <sub>oc</sub>	Draft ESG for Tier 1 (µg/g <sub>oc</sub> )	Draft ESG for Tier 2 (µg/g <sub>oc</sub> )
71432	Benzene	2.13	815.4	45.5	2.094	100	5.7
319868	BHC, delta-	3.78	43.6	2.44	3.716	230	13
58899	BHC, gamma-/Lindane	3.73	1.903 <sup>a</sup>	0.08 <sup>b</sup>	3.667	8.8	0.37
92524	Biphenyl	3.96	108.7	13.69	3.893	850	110
101553	Bromophenyl phenyl ether, 4-	5.00	27.69	1.538	4.915	2300	130
85687	Butyl benzyl phthalate	4.84	262.3	18.84	4.758	15,000	1,100
108907	Chlorobenzene	2.86	2,271	127	2.812	1,500	82
84742	Di-n-butyl phthalate	4.61	234	32.7	4.532	8,000	1,100
333415	Diazinon/Spectracide	3.7	0.1687 <sup>a</sup>	0.04329 <sup>b</sup>	3.637	0.73	0.19
132649	Dibenzofuran	4.07	366	20.4	4.001	3700	200
95501	Dichlorobenzene, 1,2-	3.43	259	1,4.39	3.372	610	34
541731	Dichlorobenzene, 1,3-	3.43	625	71.31	3.372	1,500	170
106467	Dichlorobenzene, 1,4-	3.42	183.6	15.11	3.362	420	35
60571	Dieldrin	5.37	0.2874 <sup>a,c</sup>	0.06589 <sup>b,c</sup>	5.279	55	13
84662	Diethyl phthalate	2.5	3947	220	2.458	1,100	63
115297	Endosulfan mixed isomers	4.1	0.1277	0.05059	4.031	1.4	0.54
959988	Endosulfan, alpha-	3.83	0.1277	0.05059	3.765	0.74	0.29
33213659	Endosulfan, beta-	4.52	0.1277	0.05059	4.443	3.5	1.4
72208	Endrin	5.06	0.1803 <sup>a,c</sup>	0.05805 <sup>b,c</sup>	4.974	17	5.5
100414	Ethylbenzene	3.14	6,971	389	3.087	8,500	480
67721	Hexachloroethane	4.00	211.9	11.77	3.932	1,800	100
121755	Malathion	2.89	0.8884 <sup>a</sup>	0.09671	2.841	0.62	0.067
72435	Methoxychlor	5.08	0.0962	0.0188	4.994	9.5	1.9
608935	Pentachlorobenzene	5.26	8.377	0.466	5.171	1,200	69
79345	Tetrachloroethane, 1,1,2,2-	2.39	3,698	719	2.350	830	160
127184	Tetrachloroethene	2.67	998	125	2.625	420	53
56235	Tetrachloromethane	2.73	4,375	243.1	2.684	2,100	120
108883	Toluene	2.75	3153	176	2.704	1,600	89
8001352	Toxaphene	5.50	1.903 <sup>a</sup>	0.039 <sup>b</sup>	5.407	490	10
75252	Tribromomethane/Bromoform	2.35	2,254	316.8	2.310	460	65
120821	Trichlorobenzene, 1,2,4-	4.01	699.5 <sup>a</sup>	105.1	3.942	6,100	920
71556	Trichloroethane, 1,1,1-	2.48	617	62.1	2.438	170	17
79016	Trichloroethene	2.71	4,350	465	2.664	2,000	210
108383	Xylene, <i>m</i> -	3.2	32.29	1.794	3.146	45	2.5

<sup>a</sup>FAV values.

<sup>b</sup>FCV values.

<sup>c</sup>In freshwater.

On a sediment organic carbon basis, the draft ESG,

$$ESG_{oc} (\mu g/g_{oc}) = K_{oc} (L/kg) \times [FCV, SCV] (\mu g/L) \times (10^{-3} kg_{oc}/g_{oc})$$

or

$$ESG_{oc} (\mu g/g_{oc}) = K_{oc} (L/kg) \times [FAV, SAV] (\mu g/L) \times (10^{-3} kg_{oc}/g_{oc})$$

where:

$ESG_{oc}$  = Draft ESG on a sediment organic carbon basis in  $\mu\text{g}/\text{g}_{oc}$ ;

FCV or SCV = EPA aquatic life water quality criterion final or secondary chronic value in  $\mu\text{g}/\text{L}$ ;

FAV or SAV = EPA aquatic life water quality criterion final or secondary acute value in  $\mu\text{g}/\text{L}$ ; and

$K_{oc}$  = organic carbon-water partitioning coefficient in  $\text{L}/\text{kg}$ .

$K_{oc}$  is presumed to be independent of sediment type for nonionic organic chemicals, so that the draft  $ESG_{oc}$  is also independent of sediment type. Using a site-specific organic carbon fraction,  $f_{oc}$  ( $\text{g}_{oc}/\text{g}$  sediment), the draft  $ESG_{oc}$  can be expressed as a sediment-specific value:  $ESG = (ESG_{oc}) (f_{oc})$

### *Draft Sediment Equilibrium Partitioning Sediment Guidelines (ESGs) for PAH Mixtures*

Similar to the equilibrium partitioning approach used for nonionic organics, EPA (USEPA, 2000b) has developed draft ESGs for PAH mixtures. The draft ESGs developed considers the toxicological contribution of mixtures of 34 PAHs in sediments to determine if their concentrations in any specific sediment are acceptable for the protection of benthic organisms from PAH toxicity. The equilibrium partitioning theory, the narcosis theory, and the concept of additivity (Swartz et al., 1995, Swartz, 1999) are the technical foundation for the development of draft ESGs for PAH mixtures. Because PAHs occur in sediments of different mixtures, the above approach is justified for the derivation of draft ESGs for PAHs. PAHs are considered type 1 narcotic chemicals, and the toxicities of PAHs in sediment and tissues are additive or nearly additive (Di Toro et al, 2000). Consequently, consideration of their toxicities on an individual basis may result in arriving at an under-protective guideline.

Using PAH-specific final chronic values (FCVs) or final acute values (FAVs), the effect concentration of a PAH in sediment ( $C_{oc,PAHi,FCVi}$  or  $C_{oc,PAHi,FAVi}$ ) on an organic carbon basis is calculated as the product of its FCV and  $K_{oc}$  or FAV and  $K_{oc}$ . The quotient of the organic carbon normalized sediment concentration for a specific PAH ( $C_{oc,PAHi}$ ) and the effect concentration of a PAH in sediment for a PAH-specific FCV ( $C_{oc,PAHi,FCVi}$ ) or FAV ( $C_{oc,PAHi,FAVi}$ ), is called the equilibrium partitioning sediment guideline toxic unit ( $ESGTU_{FCVi}$ ) or ( $ESGTU_{FAVi}$ ). The draft ESG for the mixture of PAHs is the sum of the  $ESGTU_{FCVi}$  or  $ESGTU_{FAVi}$  for all of the PAHs in the particular sediment. This sum is called  $\Sigma ESGTU_{FCV}$  or  $\Sigma ESGTU_{FAV}$  and is given by

$$\sum ESGTU_{FCV} = \sum ESGTU_{FCVi} = \sum \frac{C_{oc,PAHi}}{C_{oc,PAHi,FCVi}}$$

or

$$\sum ESGTU_{FAV} = \sum ESGTU_{FAVi} = \sum \frac{C_{oc,PAHi}}{C_{oc,PAHi,FAVi}}$$

Because the effect concentration of a PAH in sediment ( $C_{oc,PAHi,FCVi}$  or  $C_{oc,PAHi,FAVi}$ ) on an organic carbon basis is solubility-limited, a solubility constraint is applied to sediment concentrations when computing their individual contributions. The effect concentration is limited by the concentration in sediment organic carbon that is in equilibrium with the interstitial water at the aqueous solubility, called the maximum effect concentration  $C_{oc,PAHi,MAX}$ . Thus, only the contribution up to the maximum  $C_{oc,PAHi,MAX}$  is considered in the  $\Sigma ESGTU_{FCV}$  or  $\Sigma ESGTU_{FAV}$  analysis for PAH mixtures.

For a particular sediment, if the  $\Sigma ESGTU_{FCV}$  based on final chronic values for “total PAHs” exceeds 1.0, the station is classified as Tier 2. Similarly, if the  $\Sigma ESGTU_{FAV}$  based on final acute value exceeds 1.0, the station is classified as Tier 1. For the NSI data evaluation, most data sets reported results for only 13 PAHs. However, for this data evaluation not all 13 PAHs were required to be measured at any one station for that station to be considered for tier classification. Based on the sensitivity analysis done, it

was observed that this variation from the EPA recommended practice did not dramatically change the total number of station tier classification. Table B-2 presents the list of 13 PAHs analyzed in this *National Sediment Quality Survey* report.

**Table B-2. EPA Aquatic Life Final Acute/Chronic Values (FAV/FCV), and Effect Concentration of PAH in Sediment ( $C_{oc}$ ), Log  $K_{ow}$ , and Log  $K_{oc}$  for PAH Mixtures.**

CAS Number	Chemical Name	Log $K_{ow}$	FAV ( $\mu\text{g/L}$ )	FCV ( $\mu\text{g/L}$ )	Log $K_{oc}$	$C_{oc,PAH,FAV_i}$ ( $\mu\text{g/g}_{oc}$ )	$C_{oc,PAH,FCV_i}$ ( $\mu\text{g/g}_{oc}$ )	$C_{oc,PAH,MAX}^a$ ( $\mu\text{g/g}_{oc}$ )
83329	Acenaphthene	4.012	232.3	55.85	3.944	2,043	491	33,400
208968	Acenaphthylene	3.223	1,277	306.9	3.168	1,880	452	24,000
120127	Anthracene	4.534	86.24	20.73	4.457	2,471	594	1,300
56553	Benzo(a)anthracene	5.673	9.264	2.227	5.577	3,499	841	4,153
50328	Benzo(a)pyrene	6.107	3.982	0.9573	6.003	4,014	965	3,840
205992	Benzo(b)fluoranthene	6.266	2.818	0.6774	6.160	4,073	979	2,169
207089	Benzo(k)fluoranthene	6.291	2.669	0.6415	6.184	4,081	981	1,220
218019	Chrysene	5.713	8.495	2.042	5.616	3,511	844	826
206440	Fluoranthene	5.084	29.57	7.109	4.998	2,941	707	23,870
86737	Fluorene	4.208	163.5	39.30	4.137	2,238	538	26,000
91203	Naphthalene	3.356	805.0	193.5	3.299	1,602	385	61,700
85018	Phenanthrene	4.571	79.58	19.13	4.494	2,479	596	34,300
129000	Pyrene	4.922	42.06	10.11	4.839	2,900	697	9,090

<sup>a</sup> When the organic carbon normalized sediment concentration ( $C_{oc, PAH_i}$ ) is greater than  $C_{oc,PAH,MAX}$ , use  $C_{oc,PAH,MAX}$  in place of  $C_{oc, PAH_i}$ .

Though EPA recommends the use of 34 PAHs to derive the total draft ESG toxicity unit, some monitoring programs measure only 13 or 23 PAHs instead of a total of 34 PAHs. To determine the uncertainty in predicting the total draft ESG toxicity unit from data sets consisting of 13 or 23 PAHs, two Environmental Monitoring and Assessment Program (EMAP) data sources that measured the 34 PAHs were evaluated. Using the combined data, EPA determined the factors for the total draft ESG toxicity unit for 34 PAHs from monitoring programs that measure only 13 or 23 PAHs. The relative distribution of the equilibrium partitioning sediment guideline toxic unit with 34 PAHs ( $\Sigma\text{ESGTU}_{FCV,TOT}$ ) to the draft equilibrium partitioning sediment guideline toxic unit with 13 PAHs ( $\Sigma\text{ESGTU}_{FCV,13}$ ) is presented in Table B-3.

**Method for Determination of Log  $K_{ow}$ s.** The determination of log  $K_{ow}$  values was based on EPA draft guidelines (USEPA 2000a, b, c, d).

**Selection of Chronic Toxicity Values.** EPA developed a hierarchy of sources for chronic toxicity values for the development of the draft ESGs (USEPA, 2000e). The following sources were identified and ranked from most to least confidence in the chronic values to be used:

1. Final chronic values from the Great Lakes Initiative (GLI, 1995).
2. Final chronic values from the National Ambient Water Quality Criteria documents.
3. Final chronic values from draft freshwater criteria documents.

**Table B-3. Relative Distribution of  $\Sigma\text{ESGTU}_{FCV,TOT}$  to  $\Sigma\text{ESGTU}_{FCV,13}$  for the Combined EMAP Data Set (N = 488).**

Percentile	$\Sigma\text{ESGTU}_{FCV,TOT}^a / \Sigma\text{ESGTU}_{FCV,13}^b$
50	2.75
80	6.78
90	8.45
95	11.5
99	16.9

4. Final chronic values developed from data in EPA's Aquatic Toxicity Information Retrieval database (AQUIRE) and other sources.
5. Secondary chronic values developed from data in AQUIRE and other sources.
6. Secondary chronic values from Suter and Mabrey (1994).

When possible, draft ESGs were calculated from FCVs for aquatic life (USEPA, 1985). When FCVs could not be derived, the draft ESGs were calculated from FCVs or SCVs for aquatic life using the approach outlined in GLI (1995).

Twelve aquatic toxicity values were based on work conducted by Oak Ridge National Laboratories (Suter and Mabrey, 1994) using the GLI (1995) methodology for obtaining secondary chronic values ("Tier II"). This methodology was developed to obtain whole-effluent toxicity screening values based on all available data, but the methodology could also be used to calculate SCVs with less toxicity data than the amount required for the criteria methodology outlined in USEPA (1985). The SCVs are generally more conservative than those which can be produced by the FCV methodology, reflecting greater uncertainty in the absence of additional toxicity data. The minimum requirement for deriving an SCV is toxicity data from a single taxonomic family (Daphnidae), provided the data are acceptable. Only those values from Suter and Mabrey (1994) that included at least one daphnid test result in the calculation of the SCV were included for the *National Sediment Quality Survey*. SCVs from Suter and Mabrey (1994) were used to develop draft ESGs for the following chemicals:

benzene	ethylbenzene
chlorobenzene	1,1,2,2-tetrachloroethane
delta-BHC	tetrachloroethene
dibenzofuran	toluene
diethyl phthalate	1,1,1-trichloroethane
di-n-butyl phthalate	trichloroethene

A preliminary search of data records in EPA's AQUIRE database indicated that the following chemicals might have sufficient toxicity data for the development of FCVs or SCVs using the GLI (1995) methodology. Only diazinon had sufficient data for the development of an FCV. The other chemicals listed below had sufficient data for the development of SCVs.

biphenyl	hexachlorethane
4-bromophenyl phenyl ether	malathion
butyl benzyl phthalate	methoxychlor
diazinon	pentachlorobenzene
1,2-dichlorobenzene	tetrachloromethane
1,3-dichlorobenzene	tribromomethane
1,4-dichlorobenzene	1,2,4-trichlorobenzene
endosulfan mixed isomers	trichloromethane
alpha-endosulfan	xylene
beta-endosulfan	

In addition, EPA has developed FCVs for dieldrin and endrin (USEPA, 2000f, g).

**Calculation of Acute Toxicity Values.** Acceptable freshwater acute test results were entered in taxonomic order. If the tests were conducted properly, acute values reported as "greater than" values and those that were above the solubility of the test material were entered because rejection of such acute

values would unnecessarily lower the Final Acute Value (FAV) by eliminating acute values for resistant species. Reported results were not rounded off to fewer than four significant digits. To derive freshwater FAVs (USEPA, 1985), it was necessary to have results of acceptable acute toxicity tests with at least one species of freshwater animal in eight different families, such that all of the following minimum data requirements (MDRs) were satisfied:

1. The family Salmonidae in the Class Osteichthyes.
2. A second family in the Class Osteichthyes, preferably a commercially or recreationally important warm-water species (e.g., bluegill, channel catfish).
3. A third family in the phylum Chordata (may be in the Class Osteichthyes or may be an amphibian, etc.).
4. A planktonic crustacean (e.g., cladoceran, copepod).
5. A benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).
6. An insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).
7. A family in a phylum other than Arthropoda or Chordata (e.g., Rotifera, Annelida, Mollusca).
8. A family in any order of insect or any phylum not already represented.

In the case of a species for which at least one acceptable acute value was available, the species mean acute value (SMAV) was computed as the geometric mean of the results of all flow-through tests in which the concentrations of test material were measured. For each genus for which one or more SMAVs were available, the genus mean acute value (GMAV) was calculated as the geometric mean of the SMAVs available for the genus. The GMAVs were ranked from the highest to the lowest.

If all eight of the MDRs were satisfied, the FAV was calculated using the procedure outlined by USEPA (1985), which uses the total number of GMAVs and the four lowest. The calculated value of FAV was compared with the low SMAVs to determine whether the FAV should be lowered to protect a commercially or recreationally important species. When all eight of the acute freshwater MDRs were not satisfied, a freshwater secondary acute value (SAV) was calculated. It was essential to have at least one acceptable acute toxicity test with a species in one of the three genera (*Daphnia*, *Ceriodaphnia*, or *Simocephaus*) in the family Daphnidae.

#### *Acid-Volatile Sulfide Concentration*

EPA (USEPA, 2000c) has developed draft ESGs for metal mixtures based on their bioavailability in sediment. These guidelines are similar to the draft ESGs for nonionic organic chemicals. The draft ESGs consider cadmium, copper, lead, nickel, silver, and zinc and mixtures thereof. Solid phase and interstitial water phase draft ESGs have been developed. These draft guidelines are intended to protect benthic organisms from the direct effects of these six metals in sediments that are permanently inundated with water, are intertidal, or are inundated periodically for durations sufficient to permit development of benthic assemblages. Moreover, the draft guidelines do not consider the possibility of bioaccumulation and transfer to organisms at upper trophic levels.

The use of the total concentration of a trace metal in sediment as a measure of its toxicity and its ability to bioaccumulate is not supported by field and laboratory studies because different sediments exhibit different degrees of bioavailability for the same total quantity of metal (Di Toro et al., 1990; Luoma, 1983). These differences have been reconciled by relating organism toxic response (mortality) to the metal concentration in the sediment pore water (Adams et al., 1985; Di Toro et al., 1990). Some metals form insoluble complexes with the reactive pool of solid-phase sulfides in sediments (iron and manganese sulfides), restricting their bioavailability. AVS has been used for divalent cationic metals to predict their bioavailability in sediments. The metals that can bind to these sulfides have sulfide solubility parameters smaller than those of iron sulfide, and they include nickel, zinc, cadmium, copper,

lead, and mercury. In addition, more recently Berry et al. (1999) used AVS to predict the toxicity of sediments spiked with silver. However, silver is different from divalent transition metals because it predominantly exists as monovalent and 2 moles of silver are required to bind to 1 mole of sulfide. In this NSI data evaluation, silver has been added to other metals (cadmium, copper, lead, nickel, and zinc) in sediment AVS assessment.

Acid-volatile sulfide (AVS) is one of the major chemical components that control the activities and availability of metals in the pore waters of anaerobic sediments (Meyer et al., 1994). Because binding factors other than AVS dominate the bioavailability, the SEM - AVS methodology for predicting the bioavailability and toxicity of selected metals is valid only in anaerobic sediments (Berry et al., 1996). AVS is operationally defined as the sulfide fraction consisting of solid metal sulfide, mainly in the form of iron monosulfide (Hansen et al., 1996a). The metal concentrations extracted during the same analysis are called the simultaneously extracted metals (SEM). SEM is operationally defined as those metals that form less soluble sulfides than do iron or manganese (i.e., the solubility products of these sulfides are lower than that of iron or manganese sulfide) and that are at least partially soluble under the same test conditions in which the AVS content of the sediment is determined (Allen et al., 1993; Di Toro et al., 1992; Meyer et al., 1994).

Laboratory studies using spiked sediments and field-collected metal-contaminated sediments demonstrated that when the molar ratio of SEM to AVS,  $[SEM]/[AVS]$ , was less than 1 (excess AVS remained), no acute toxicity (mortality greater than 50 percent) was observed in any sediment for any benthic test organism. When  $[SEM]/[AVS]$  was greater than 1 (excess metal remained), the mortality of sensitive species (e.g., amphipods) increased in the range of 1.5 to 2.5  $\mu\text{mol}$  of SEM per  $\mu\text{mol}$  AVS (Casas and Crecelius, 1994; Di Toro et al., 1992).

Experimental studies indicate that the lower limit of applicability for AVS is approximately 1 mmol AVS/g sediment and possibly lower; other sorption phases, such as organic carbon, probably become important for sediments with smaller AVS concentrations and for metals with large partition coefficients and large chronic water quality criteria (Di Toro et al., 1990). In addition, studies indicate that copper, as well as mercury, might be associated with another phase in sediments, such as organic carbon, and AVS alone might not be the appropriate partitioning phase for predicting its toxicity. Pore-water concentrations of metals should also be evaluated (Allen et al., 1993; Ankley et al., 1993; Casas and Crecelius, 1994). The AVS approach has been traditionally used to predict when a sediment contaminated with metals is not acutely toxic (Ankley et al., 1993; Di Toro et al., 1992). However, Hansen et al. (1996b) studied the chronic effect of cadmium in sediments and concluded that the equilibrium partitioning-based SEM-AVS analysis may be used for chronically exposed benthic organisms.

### *Logistic Regression Model Approach*

The sediment chemistry screening values used to evaluate the NSI data for potential adverse effects of sediment contamination on aquatic life include both theoretically and empirically based values. The theoretically based values rely on physical/chemical properties of sediment and chemicals to derive concentrations of a substance (or substances in the case of metals mixtures and PAH mixtures) that are protective to benthic aquatic life. The theoretically based screening values include the draft equilibrium partitioning sediment guidelines for nonionic organics, metal mixtures, and PAH mixtures. The empirically based, or correlative, screening values rely on paired field and laboratory data to relate incidence of observed biological effects to the dry-weight sediment contamination of a specific chemical. The empirically based, correlative screening values include the effects range-median (ERM)/effects range-low (ERL) values, probable effects level (PEL)/threshold effects level (TEL), and apparent effects thresholds (AET). Field et al. (1999, 2001 [in press]) have proposed an alternative empirical method for evaluating sediment quality by using logistic regression models. These models can be used to predict the probability of observing specific toxic effects.

The logistic model was originally developed for use in survival analysis, where the dependent variable of interest has only two outcomes—toxic or nontoxic—and hence can be represented by a binary indicator variable taking on values of 0 and 1.

For a single independent variable ( $x$ ), the logistic regression model can be expressed in the following form:

$$p = \frac{\exp[B_0 + B_1(x)]}{1 + \exp[B_0 + B_1(x)]}$$

where  $p$  = probability of observing a toxic effect,  $B_0$  = intercept parameter,  $B_1$  = slope parameter, and  $x$  = chemical concentration in  $\log_{10}$  units. Metal concentrations are expressed in parts per million (ppm) and concentrations of organics are in parts per billion (ppb) in the preceding equation.

Field et al. (1999) used matched sediment chemistry and toxicity data obtained from sources spanning many geographic areas and toxicity endpoints. From the database, separate tables were created for individual contaminants. The individualized tables contained chemical concentrations for each sample, with the toxicity results indicating whether the sample was toxic or nontoxic for each toxicity endpoint. Samples classified as toxic were screened to eliminate the possibility of a selected contaminant's not contributing to the reported toxic effect. Within the same study and geographical area, the concentration of a particular contaminant was compared to the mean concentration of the same contaminant identified as nontoxic. When the concentration in a toxic sample was less than or equal to the mean concentration in a nontoxic sample, the samples were excluded from the data set used to develop the logistic model for the particular chemical. These models were developed using 10-day amphipod survival toxicity tests with marine and estuarine data. Samples were considered toxic if they were significantly different from a negative control—as designated by the original investigator—and had less than 90 percent survival.

The screening procedure developed by the authors enabled the data to be transformed into a format consistent with logistic regression modeling. For preselected concentration intervals—based on the range of sample concentrations for each contaminant—the proportion of toxic samples was computed. Using the screened data, individual logistic regression models were developed for each contaminant, and the slope ( $B_1$ ), intercept ( $B_0$ ), and chi-square statistic values were calculated using the maximum likelihood approach. Similar to the correlation coefficient ( $r$ ) in linear regression models, the chi-square statistic provides information on the slope parameter ( $B_1$ ) of the logistic regression model and the goodness-of-fit of the model with the data. For data sets with comparable sample sizes, a larger chi-square indicates a goodness-of-fit between the logistic model and the data used to derive the model. Since the chi-square statistic increases with sample size, the normalized chi-square statistic value, i.e., chi-square divided by the sample size, is more applicable when data sets of different magnitude are considered.

Although the logistic model developed gives the probability of observing a toxic effect for a particular contaminant concentration, the model can also be inverted to determine the concentrations at which a certain percentage of the samples would be deemed toxic. When the model is used in the inverse form, it is also possible to calculate the confidence interval for the probability of finding a percentage of the samples toxic at a particular concentration. The confidence interval reflects the range of concentrations within which a certain percentage of toxic effect can be expected.

Table B-4 gives the intercept coefficients, the slope, the number of samples used to derive the individual chemical-specific logistic regression model, and the normalized chi-square value for a list of 37 chemicals representing metals, PAHs, and PCBs. The log chemical concentrations, normalized to either dry weight or total organic carbon, are in parts per million (ppm) for metals and are in parts per billion (ppb) for organics.

**Table B-4. Logistic Regression Model Coefficients (Field et al., 2001 [in press]).**

CAS Number	Chemical Name	Intercept (B <sub>0</sub> )	Slope (B <sub>1</sub> )	No. of Samples	Normalized $\chi$ -square Value
83329	Acenaphthene	-3.6165	1.7532	1,424	0.334
208968	Acenaphthylene	-2.962	1.3797	1,447	0.23
120127	Anthracene	-3.6574	1.4854	1,823	0.289
7440360	Antimony	-0.9005	2.4111	1,718	0.25
7440382	Arsenic	-4.1407	3.1674	2,336	0.173
56553	Benz(a)anthracene	-4.2013	1.5747	2,099	0.298
50328	Benzo(a)pyrene	-4.3005	1.5832	2,053	0.299
205992	Benzo(b)fluoranthene	-4.5409	1.4916	1,348	0.266
191242	Benzo(g,h,i)perylene	-4.2811	1.5878	1,818	0.25
207089	Benzo(k)fluoranthene	-4.2781	1.5669	1,376	0.286
92524	Biphenyl	-4.1144	2.2085	1,226	0.263
7440439	Cadmium	-0.34	2.5073	2,413	0.313
7440473	Chromium, total	-6.4395	2.9952	2,399	0.195
218019	Chrysene	-4.3241	1.5372	2,126	0.286
7440508	Copper	-5.7878	2.9325	2,580	0.383
53703	Dibenz(a,h)anthracene	-3.6308	1.7692	1,546	0.326
60571	Dieldrin	-1.1728	2.558	633	0.354
581420	Dimethylnaphthalene, 2, 6-	-4.0456	1.904	1,249	0.201
206440	Fluoranthene	-4.4574	1.4787	2,189	0.263
86737	Fluorene	-3.7146	1.8071	1,668	0.323
193395	Indeno(1,2,3-c,d)pyrene	-4.3674	1.6245	1,837	0.269
7439921	Lead	-5.4523	2.7662	2,481	0.274
7439976	Mercury	0.8041	2.5461	2,296	0.32
91576	Methylnaphthalene, 2-	-3.7579	1.7833	1,704	0.25
90120	Methylnaphthalene, 1-	-4.1405	2.0961	1,368	0.239
832699	Methylphenanthrene, 1-	-3.5884	1.7501	1,401	0.284
91203	Naphthalene	-3.7753	1.6152	1,816	0.235
7440020	Nickel	-4.6119	2.7658	2,450	0.18
72548	p,p'-DDD	-1.8983	1.4913	1,360	0.268
72559	p,p'-DDE	-1.8392	0.9129	1,552	0.162
50293	p,p'-DDT	-1.7705	1.6786	931	0.335
1336363	PCBS, total	-3.1939	1.196	1,617	0.241
198550	Perylene	-4.6827	1.7632	1,823	0.218
85018	Phenanthrene	-4.4576	1.6768	2,173	0.298
129000	Pyrene	-4.708	1.5854	2,240	0.287
7440224	Silver	-0.1117	1.9684	2,103	0.252
7440666	Zinc	-7.9834	3.342	2,516	0.279

Using the logistic model developed for each contaminant, the probability of observing a toxic effect is computed for various chemical concentrations (Field et al., 1999, 2001 [in press]). By tabulating the probability of toxic effects, a maximum value can be computed for the list of chemicals considered.

For the unscreened data, the proportion of toxic samples—within different ranges of maximum probability of toxic effects computed above at discrete concentration intervals—is determined as the ratio of the number of toxic samples to the total number of samples in the (unscreened) data. This procedure can be repeated for different concentrations of the individual contaminants to obtain sufficient data to generate a regression equation with the proportion of toxic samples as the dependent variable and the maximum probability of observing toxic effects as the independent variable. The following regression equation (Field et al., 2001 [in press]) was used in the NSI data evaluation:

$$y = 0.11 + 0.33 p_{\max} + 0.4 p_{\max}^2$$

where  $p_{\max}$  = maximum probability of observing a toxic effect and  $y$  = predicted proportion toxic.

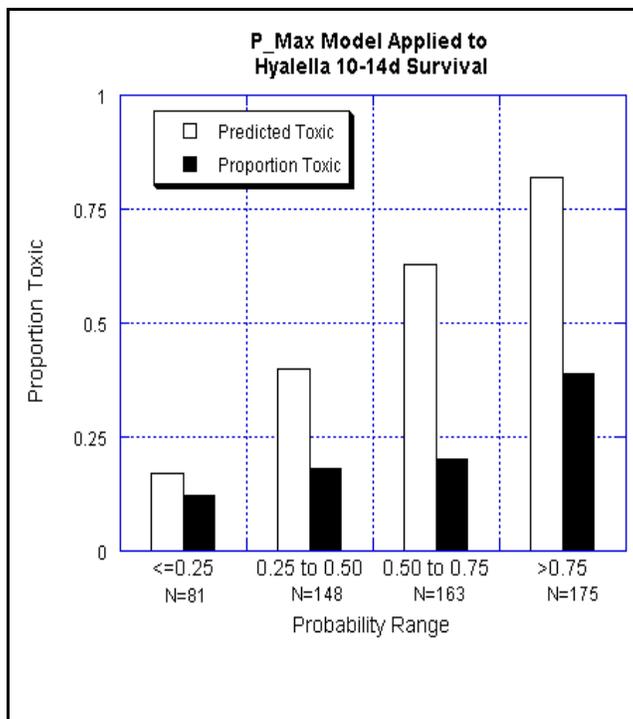
From multiple chemical measures of the 37 target chemicals, the predicted proportion toxic is computed for each sample using the preceding regression equation. When the maximum value of the predicted proportion toxic is greater than or equal to 50 percent (0.5), the station is classified as Tier 1. When the maximum value of the predicted proportion toxic is less than 50 percent but greater than or equal to 25 percent, the stations are classified as Tier 2. All other stations with available data are grouped as Tier 3.

To evaluate the applicability of the marine amphipod models to freshwater data, matching sediment chemistry and toxicity data were compiled for three freshwater toxicity test endpoints: 10- to 14-day acute lethality tests with *Hyaella azteca* and *Chironomus* spp. and a long-term 28-day growth and survival test with *H. azteca*. The predicted proportion toxic from the marine models was compared to the observed acute toxicity for each test endpoint within four probability quartiles. The results of the evaluations for all three endpoints showed that the increase in probability of toxicity based on the marine amphipod model was accompanied by an increase in the observed proportion toxic. For the acute freshwater tests with *H. azteca* and *Chironomus* spp., only samples that were predicted by the model to have a high probability of toxicity ( $p > 0.75$ ) showed an increase in the proportion of samples that were toxic (Figure B-1; *Chironomus* plot not shown). However, the results for the chronic *H. azteca* test endpoint (28-day growth and survival) correspond very well to the model predictions (Figure B-2). In the 28-day database, 61 samples had a predicted proportion toxic greater than 0.5 (with a mean of 0.68) compared to 0.61 observed proportion toxic. These results indicate that the LRM P\_Max model used in this analysis would tend to overestimate toxicity observed in *H. azteca* and *Chironomus* spp. 10- to 14-day survival tests, but not the *H. azteca* 28-day growth and survival test. Based on this evaluation, the difference between model predictions and the acute freshwater toxicity test results may be more related to differences in endpoint sensitivity than to differences between marine and freshwater geochemistry.

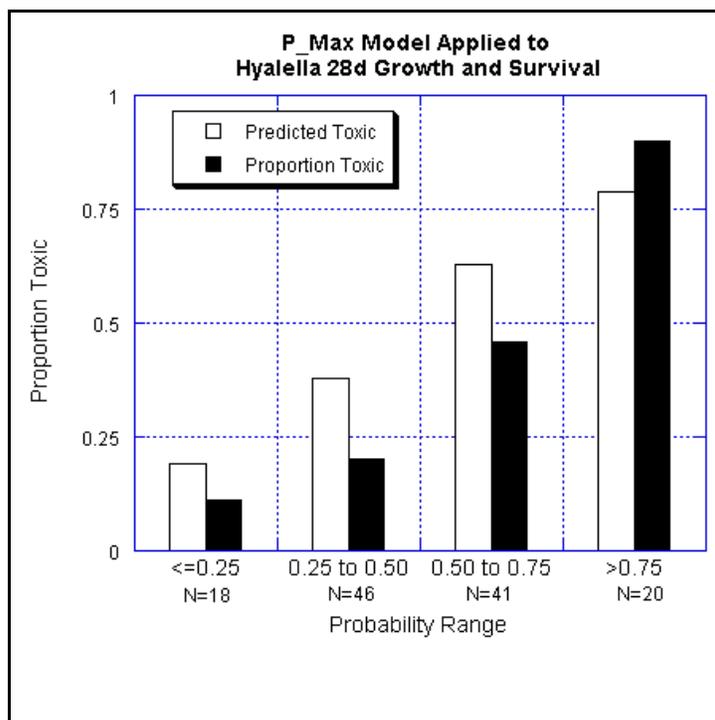
### *Sediment Toxicity Approaches*

Sediment toxicity tests provide important information on the effects of multiple chemical exposures to assist in the evaluation of sediment quality. Methods for testing the short- and long-term toxicity of sediment samples to benthic freshwater and marine organisms have been developed (see reviews in API, 1994; Burton et al., 1992; Lamberson et al., 1992; USEPA, 1994a, b, 2000h) and used primarily for dredged material evaluation (USEPA and USACE, 1994). The NSI data contain short- and long-term sediment toxicity results from tests in which organisms were exposed to field-collected sediments and mortality or other endpoints were recorded.

Data in the NSI database were reviewed, and only bulk sediment nonmicrobial toxicity tests with test durations of 7 days or more were analyzed. Test results with survival (or mortality) as an endpoint were considered for all marine and freshwater species with valid control-adjusted results. In addition, for freshwater species growth-based endpoints—length and weight—were considered for long-term toxicity. Test results with the freshwater invertebrate *Hyaella* were analyzed for variation in control-adjusted length. Variations in control-adjusted weight were considered for the freshwater invertebrates *Hyaella*



**Figure B-1. Application of the logistic model to freshwater data for *Hyalella* 10- to 14-day survival endpoint.**



**Figure B-2. Application of logistic model to freshwater data for *Hyalella* 28-day growth and survival endpoint.**

and *Chironomus*. Test results with either unknown test species or unknown test duration were not analyzed in this NSI data evaluation. Table B-5 presents a list of species used in toxicity tests whose results are included in the *National Sediment Quality Survey*.

**Table B-5. Species Used in Bulk Sediment Toxicity Tests<sup>a</sup>**

<b>Survival (or Mortality) Endpoint: Marine and Freshwater Species</b>		
<i>Acanthomysis costata</i>	<i>Gammarus lacustris</i>	<i>Neanthes</i> spp.
<i>Acanthomysis macropsis</i>	<i>Grandidierella japonica</i>	<i>Nebalia pugettensis</i>
<i>Ampelisca abdita</i>	<i>Helisoma</i> spp.	<i>Nephtys caecoides</i>
<i>Ampelisca verrilli</i>	<i>Hexagenia limbata</i>	<i>Nereis virens</i>
<i>Armandia brevis</i>	<i>Hexagenia</i> spp.	<i>Oncorhynchus mykiss</i>
<i>Ceriodaphnia dubia</i>	<i>Holmesimysis sculpta</i>	<i>Palaemonetes pugio</i>
<i>Chironomus riparius</i>	<i>Hyalella azteca</i>	<i>Panaeus duorarum</i>
<i>Chironomus tentans</i>	<i>Lepidactylus dytiscus</i>	<i>Panope generosa</i>
<i>Corophium acherusicum</i>	<i>Leptocheirus plumulosus</i>	<i>Pimephales promelas</i>
<i>Corophium spinicorne</i>	<i>Limnodrilus hoffmeisteri</i>	<i>Pontoporeia hoyi</i>
<i>Corophium volutator</i>	<i>Lumbriculus variegatus</i>	<i>Protothaca staminea</i>
<i>Crangon</i> spp.	<i>Lytechinus pictus</i>	<i>Rhepoxynius abronius</i>
<i>Crassostrea virginica</i>	<i>Macoma nasuta</i>	<i>Rhepoxynius hudsoni</i>
<i>Daphnia magna</i>	<i>Metamysidopsis elongata</i>	<i>Streblospio benedicti</i>
<i>Dendraster excentricus</i>	<i>Mysidopsis bahia</i>	<i>Strongylocentrotus purpuratus</i>
<i>Diporeia</i> spp.	<i>Mytilus edulis</i>	<i>Stylodrilus heringianus</i>
<i>Eohaustorius estuarius</i>	<i>Neanthes arenaceodentata</i>	
<b>Growth-Based Endpoint (Length): Freshwater Species</b>		
<i>Hyalella azteca</i>		
<b>Growth-Based Endpoint (Weight): Freshwater Species</b>		
<i>Chironomus riparius</i>	<i>Chironomus tentans</i>	<i>Hyalella azteca</i>

<sup>a</sup> With test durations  $\geq$  7 days.

**Test Controls.** Toxicity data were screened to determine whether control data were reported. Sediment toxicity test laboratory or performance controls are usually clean sand or sediment tested under the same conditions in which the test organisms are exposed at the same time as those exposed to the sediment samples tested. Controls are used to determine whether observed mortality might be the result of the quality of test organisms used or other factors, and not the result of exposure to possible toxics in the sediment samples.

The databases were screened to locate control test data for each sediment sample tested. Multiple control sample test results were reported in some of the databases. These were determined to be replicate test results. The percent survival (or mortality) for the reference replicates were averaged for each reference site to obtain the mean percent survival (or mortality).

The control-corrected results were obtained using the following equation:

$$\frac{\text{percent survival of organisms in sample test}}{\text{percent survival of organisms in control test}} = \text{control-corrected percent survival}$$

$$\text{percent survival of organisms in sediment sample test} = \frac{\text{control-corrected percent survival} \times \text{percent survival of organisms in control test}}{100}$$

Results of control tests reported as “percent mortality” were converted to “percent survival” by the following calculations:

$$\text{percent survival} = 100 - \text{percent mortality}$$

$$\text{percent survival} = \frac{\text{number of surviving organisms}}{\text{total number of organisms in test}}$$

**Determination of Thresholds for Tier Classification.** Minimum detectable differences (MDDs) based on sediment toxicity data from round robin tests, were used to determine the thresholds for tier classification of toxicity data (USEPA, 2000h). Although the quantitative relationship between statistical significance and expected ecological effects is not fully understood, we presume that these values are related to expected ecological effects as is the presumption of other EPA assessment approaches (USEPA, 1985). Table B-6 shows the MDDs calculated for the different species and test endpoints. MDD values from a control sediment are compared with contaminated sediments used in round robin 10-day and 28-day tests. The MDDs were calculated with a one-tailed *t*-test at a confidence level of 95 percent with four replicates. Based on the values of MDDs presented in Table B-6, samples with a percent reduction of mean MDD plus 2 standard deviations from control data (selected 25 percent mortality from a range of 25.0 to 29.8 percent mortality, i.e., < 75 percent control-adjusted survival) were classified as Tier 1 for survival endpoints. Similarly when the percent reduction from the control data was mean MDD less one standard deviation (i.e., < 90 percent control-adjusted survival), the samples with survival endpoints were categorized as Tier 2.

Using the threshold stated above, for growth-based measurements of length, samples with less than 90 percent control-adjusted length were classified as Tier 1 and samples with less than 70 percent control-adjusted weight were classified as Tier 1. Tier 2 classification for length was based on less than 95 percent control-adjusted length and less than 90 percent control-adjusted weight.

**Table B-6. Minimum Detectable Differences (MDDs) Calculated from Round Robin Test Data**

Species/Endpoint		Average MDD (% reduction from control)	Standard Deviation (as % of control)	Mean +2 SD (% reduction from control)	Mean - 1 SD (% reduction from control)
<i>Chironomus tentans</i> 10-d Survival	WBS <sup>a</sup> vs LS <sup>b</sup>	13.7	7.2	28.1	6.5
	WBS vs DC <sup>c</sup>	13.3	5.9	25.0	7.4
<i>Hyalella azteca</i> 10-d Survival	WBS vs LS	15.8	5.1	26.1	10.7
	WBS vs DC	16.6	6.6	29.8	10.0
<i>Hyalella azteca</i> 28-d Length	WBS vs LS	4.9	1.1	7.1	3.9
	WBS vs CC <sup>d</sup>	5.3	1.1	7.5	4.2
<i>Chironomus tentans</i> 10-d Weight	WBS vs LS	12.3	5.1	22.5	7.2
	WBS vs DC	19.6	5.8	31.2	13.9
<i>Hyalella azteca</i> 28-d Weight	WBS vs LS	17.6	7.1	31.8	10.5
	WBS vs CC	27.3	11.1	49.5	16.2

<sup>a</sup>WBS: control sediment from West Bearskin Lake, MN

<sup>b</sup>LS: contaminated sediments from Little Scioto River, OH.

<sup>c</sup>DC: contaminated sediments from Defoe Creek site, MI.

<sup>d</sup>CC: contaminated sediments from Cole Creek, MI.

### ***Human Health Assessments***

In the evaluation of NSI data, two primary evaluation parameters were used to assess potential human health impacts from sediment contamination: (1) sediment chemistry theoretical bioaccumulation potential and (2) tissue levels of contaminants in demersal, nonmigratory, and edible species.

#### ***Theoretical Bioaccumulation Potential***

The theoretical bioaccumulation potential (TBP) is an estimate of the equilibrium concentration of a contaminant in tissues if the sediment in question were the only source of contamination to the organism (USEPA and USACE, 1994). The TBP calculation is used as a screening mechanism to represent the magnitude of bioaccumulation likely to be associated with nonpolar organic contaminants in the sediment. At present, the TBP calculation can be performed only for nonpolar organic chemicals; however, methods for TBP calculations for metals and polar organic chemicals are under development (USEPA and USACE, 1994).

The environmental distribution of nonpolar organic chemicals is controlled largely by their solubility in various media. Therefore, in sediments they tend to occur primarily in association with organic matter (Karickhoff, 1981) and in organisms they are found primarily in the body fats or lipids (Bierman, 1990; Geyer et al., 1982; Konemann and van Leeuwen, 1980; Mackay, 1982). Bioaccumulation of nonpolar organic compounds from sediment can be estimated from the organic carbon content of the sediment, the lipid content of the organism, and the relative affinities of the chemical for sediment organic carbon and animal lipid content (USEPA and USACE, 1994). It is possible to relate the concentration of a chemical in one phase of a two-phase system to the concentration in the second phase when the system is in equilibrium. The TBP calculation focuses on the equilibrium distribution of a chemical between the sediment and the organism. By normalizing nonpolar organic chemical concentration data for lipid in organisms, and for organic carbon in sediment, it is possible to estimate the preference of a chemical for one phase or the other (USEPA and USACE, 1994).

The TBP can be calculated relative to the biota-sediment accumulation factor (BSAF), as in the following equation (USEPA and USACE, 1994):

$$\text{TBP} = \text{BSAF} (C_s/f_{oc})f_i$$

where TBP is expressed on a whole-body basis in the same units of concentration as  $C_s$  and

TBP = theoretical bioaccumulation potential (ppm);

$C_s$  = concentration of nonpolar organic chemical in sediment (ppm);

BSAF = biota-sediment accumulation factor (ratio of the concentration of a chemical in tissue, normalized to lipid, to the concentration of the chemical in surface sediment, normalized to organic carbon (in kg sediment organic carbon/kg lipid));

$f_{oc}$  = total organic carbon (TOC) content of sediment expressed as a decimal fraction (i.e., 1 percent = 0.01); and

$f_i$  = organism lipid content expressed as a decimal fraction (e.g., 3 percent = 0.03) of fillet or whole-body dry weight.

BSAF values used in the TBP evaluation were extracted from USEPA (1997). If TOC measurements were not available at a site,  $f_{oc}$  was assumed to be 0.01 (1 percent).

For the evaluation of NSI data, EPA selected a 3 percent lipid content in fish fillets for the TBP calculation for assessing human health effects from the consumption of contaminated fish. Lipid normalization is now part of the EPA guidance on bioaccumulation, and the current national methodology uses a 3 percent value for human health assessments. *The Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors* (USEPA, 1995) uses a 3.10 percent lipid value for trophic level 4 fish and 1.82 percent for trophic level 3 fish in its human health assessments.

As part of the NSI data TBP evaluation, EPA also evaluated percent lipid measurements included in the STORET database, the *National Study of Chemical Residues in Fish* (NSCRF; USEPA, 1992b), and other published sources and compared those values to the value selected for the NSI data evaluation (Appendix C of EPA-823-R-97-006). The mean fillet percent lipid content for various groups of fish species in the STORET database ranged from 0.753 to 4.49 percent; in the NSCRF, mean fillet values ranged from 1.6 to 4.9 percent. The mean whole-body percent lipid content for various groups of fish species in the STORET database ranged from 3.757 to 6.33 percent; in the NSCRF, mean whole-body values ranged from 4.6 to 8.8 percent.

In the NSI data evaluation approach, TBP values were compared to U.S. Food and Drug Administration (FDA) tolerance/action/guidance levels and EPA risk levels. These parameters are discussed below.

#### *FDA Tolerance/Action/Guidance Levels*

FDA is responsible for the safety of the Nation's commercial food supply, including fish and shellfish, for human consumption. Under the authority of the Federal Food, Drug and Cosmetic Act (FFDCA), FDA ensures that regulated products are safe for use by consumers. The FFDCA authorizes FDA to conduct assessments of the safety of ingredients in foods. The key element of the FFDCA, and the source of FDA's main tools for enforcement, is the prohibition of the "adulteration" of foods. FDA can prescribe the level of contaminant that will render a food adulterated and, therefore, can initiate enforcement action based on scientific data. The establishment of guidance and action levels (informal judgments about the level of a food contaminant to which consumers can be safely exposed) or tolerances (regulations having the force of law) is the regulatory procedure FDA uses to control environmental contaminants in the commercial food supply.

During the 1970s the available detection limits were considered to demonstrate elevated contamination and were used as action levels. Since that time FDA has focused on using risk-based standards derived by individually considering each chemical and the species of fish it is likely to contaminate. FDA also considered (1) the amount of potentially contaminated fish eaten and (2) the average concentrations of contaminants consumed. FDA has established action levels in fish for 10 pesticides and methylmercury, tolerance levels for polychlorinated biphenyls (PCBs), and guidance for 5 metals.

### *EPA Risk Levels*

Potential impacts on humans are evaluated by estimating potential carcinogenic risks and noncarcinogenic hazards associated with the consumption of chemically contaminated fish tissue. In this assessment it was assumed that the only source of contamination to fish is contaminated sediment. The procedures for estimating human health risks due to the consumption of chemically contaminated fish tissue are based on *Risk Assessment Guidance for Superfund* (USEPA, 1989) and *Guidance for Assessing Chemical Contamination Data for Use in Fish Advisories, Volume II: Development of Risk-Based Intake Limits* (USEPA, 1994c).

EPA human health risk assessment methods were used in this assessment to determine the levels of contamination in fish that might result in a  $10^{-5}$  cancer risk (1 in 100,000 extra chance of cancer over a lifetime) or a noncancer hazard in humans. A  $10^{-5}$  risk level exceeds the lower bound ( $10^{-6}$ ) but is lower than the upper bound ( $10^{-4}$ ) of the risk range accepted by EPA (USEPA, 1990).

Human health cancer risks and noncancer hazards are based on the calculation of the chronic daily intake (CDI) of contaminants of concern:

$$CDI = \frac{(EPC)(IR)(EF)(ED)}{(BW)(AT)}$$

where:

- CDI = chronic daily intake (mg/kg/day);
- EPC = exposure point concentration (contaminant concentration in fish);
- IR = ingestion rate (6.5 g/day);
- EF = exposure frequency (365 days/year);
- ED = exposure duration (70 years);
- BW = body weight (70 kg); and
- AT = averaging time (70 years x 365 days/year).

These are the same parameter values EPA used to develop human health water quality criteria. Carcinogenic risks are then quantified using the equation below:

$$\text{Cancer risk}_i = (CDI) (SF_i)$$

where:

- Cancer risk<sub>i</sub> = the potential carcinogenic risk associated with exposure to chemical *i* (unitless);
- CDI<sub>i</sub> = chronic daily intake for chemical *i* (mg/kg/day); and
- SF<sub>i</sub> = slope factor for chemical *i* (mg/kg/day)<sup>-1</sup>.

The hazard quotient, which is used to quantify the potential for an adverse noncarcinogenic effect to occur, is calculated using the following equation:

$$HQ_i = \frac{CD_i}{RfD_i}$$

where:

HQ<sub>i</sub> = hazard quotient for chemical *i* (unitless);

CD<sub>i</sub> = chronic daily intake for chemical *i* (mg/kg/day); and

RfD<sub>i</sub> = reference dose for chemical *i* (mg/kg/day).

If the hazard quotient exceeds unity (i.e., 1), an adverse health effect might occur. The higher the hazard quotient, the more likely that an adverse noncarcinogenic effect will occur as a result of exposure to the chemical. If the estimated hazard quotient is less than unity, noncarcinogenic effects are unlikely to occur.

Using these formulas, the fish tissue concentration (EPC) of a contaminant that equates to a cancer risk of 10<sup>-5</sup> or a hazard quotient that exceeds unity can be back-calculated.

Cancer risk:

$$EPC = \frac{(10^{-5})(BW)(AT)(C_1)}{(IR)(EF)(ED)(SF_i)}$$

Noncancer hazard:

$$EPC = \frac{(BW)(AT)(RfD_i)(C_1)}{(IR)(EF)(ED)}$$

where:

C<sub>1</sub> = conversion factor (10<sup>3</sup> g/kg).

The cancer slope factors and noncancer reference doses used in the previous *National Sediment Quality Survey* report to Congress (Appendix E, Table E-1, USEPA, 1997) were used to calculate the EPA risk levels and hazard quotients used in this NSI data evaluation.

### *Tissue Levels of Contaminants*

In addition to sediment chemistry TBP values, measured levels of contaminants in the tissues of resident aquatic species were used to assess potential human health risk. As was the case with the evaluation of TBP values, the NSI data evaluation approach compared contaminant tissue levels to FDA tolerance/action/guidance levels and EPA risk levels. Each of these parameters was discussed in the previous section. In such a comparison it is assumed that contaminant concentrations in tissue result from bioaccumulation of contaminants in the sediment.

The draft ESGs used for the NSI data evaluation for nonionic organics, PAH mixtures, metal mixtures, model parameters used for the logistic regression models, EPA risk levels and FDA tolerance/action/guidance levels are presented in Table C-1 of Appendix C.

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