

**Quality Assurance Project Plan under Task Order SMAVCS3
WRS Number 0.52.1.204.005.000
TDD 2-04: Scientific Support for CEAM
Model Design, Development, Support, and Maintenance
Project Title: AQUATOX**

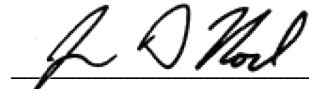
CSRA LLC (CSRA) and sub-contractor Warren Pinnacle Consulting, Inc. (WPC) prepared this Quality Assurance Project Plan (QAPP) under WRS Number 0.52.1.204.005.000, as a project-specific task. The work request involves model development, updates to model documentation, and also provides technical user support.

This QAPP ensures the quality of model development that is required to complete the work-request tasks.

This QAPP is based closely on a 2012 EPA-Approved QAPP for “Technical Support Activities for AQUATOX” under contract EP-C-12-006. The following EPA guidance documents were also consulted: *Guidance for Quality Assurance Project Plans* (EPA QA/G-5, 2002), *Guidance for Quality Assurance Project Plans for Modeling* (EPA QA/G-5M, 2002), and *QAPP Requirements for Secondary Data Research Projects* (1999).

A. Project Management

A1. Title and Approval Sheet



U.S. EPA Quality Assurance Coordinator, James Noel
10/18/2016
Date



U.S. EPA Project Officer, Rajbir Parmar
10/5/2016
Date

Brenda Rashleigh


U.S. EPA Principal Investigator, Brenda Rashleigh
10/5/2016
Date



CSRA LLC (CSRA) Program Manager, Deborah Miller
10/5/2016
Date

 for

CSRA LLC (CSRA) TDD Lead, Henry Helgen
10/5/2016
Date



CSRA Quality Assurance (QA) Lead, Marguerite Jones
10/5/2016
Date

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A3. Distribution List

A copy of this QAPP was distributed to the following individuals:

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Mr. Jonathan Clough, Sub-contractor, WPC, (802) 496-3476.
Dr. Marco Propato, Sub-contractor, WPC, (802) 496-5581.

A4. Project Organization

The principal CSRA and sub-contractor staff members are presented in the organizational chart below (Figure 1).

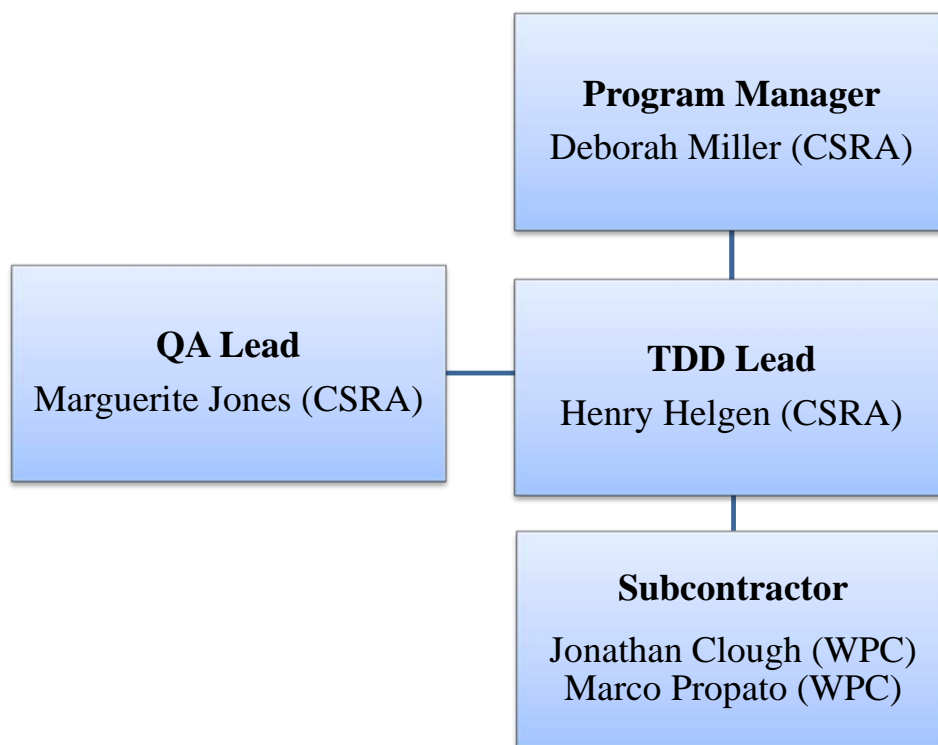


Figure 1. Project Personnel Organizational Diagram

The principal staff members' responsibilities are presented in Table 1.

Table 1. Principal Staff Responsibilities

Title	Name	Responsibility	Contact Information
Program Manager	Deborah Miller	Directs all program activities and provides oversight of the Work Assignment.	703-461-2040 deborah.miller@csra.com
TDD Lead	Henry Helgen	Oversees all activities related to the Work Plan. Approves technical modifications, documentation, and final products. Manages sub-contractors. Ensures that all elements of the project follow QA procedures in the QAPP.	218-529-5140 helgen.henry@epa.gov henry.helgen@csra.com

Title	Name	Responsibility	Contact Information
QA Lead	Marguerite Jones	Assists with the QAPP and evaluates project personnel adherence to the QAPP.	703-461-2247 maggie.jones@csra.com
Sub-contractor	Jonathan Clough	Assists with QAPP development. Performs and supervises all sub-contracting activities including model programming, documentation, adherence to this QAPP, and interaction with users.	(802) 496-3476 jclough@warrenpinnacle.com
Sub-contractor	Marco Propato	Performs model development, documentation, model testing, and code verification.	(802) 496-5581 mpropato@warrenpinnacle.com

A5. Problem Definition/Background

The ecosystem model, AQUATOX, developed by Dr. Richard Park of Eco Modeling (retired) and Jonathan Clough of Warren Pinnacle Consulting, Inc. (WPC), models the combined environmental fate and effects of many environmental stressors in aquatic ecosystems. The model was first released by EPA's Office of Science & Technology (OST) in 2000, and Release 1.1 was distributed in 2001. AQUATOX was successfully peer reviewed by a panel convened for EPA's Office of Water (OW) and Office of Pollution Prevention and Toxics (OPPT). In early 2004 Release 2 was issued. In 2005 Release 2.1 was issued and Release 2.2 followed in 2006. Release 3, which has many additional capabilities, completed EPA peer review and was issued in August 2009. [Release 3.1](#), which improves 64 bit compatibility and includes an anadromous fish module, was released by EPA in August 2012. [Release "3.1 plus"](#) includes nutrient limitation in plants based on internal rather than external nutrients and was released by EPA in April 2014.

AQUATOX consists of extensive object-oriented Pascal code developed in the Delphi programming system. The full Pascal code is protected by an open-source license and is provided under the terms of this TDD. The model consists of numerous differential equations that draw on site characteristics and state-variable parameters contained in a "study" file. The model also has associated parameter and site-characteristic databases that can be linked to a study. State-variable output can be tabulated and graphed by the model; rates and limitations to photosynthesis can also be saved and output as tables and graphs. The results of a simulation with all the boundary conditions, such as site constants and parameter values, can be saved as a text file for archival purposes. The model is described more fully in the appended Work Plan. All model equations, parameters, and references are documented in the Release 3.1 plus *Technical Documentation* ([Park and Clough, April 2014](#)); and model usage is described in the Release 3.1 plus *User's Manual* ([Clough, April 2014](#)).

Numerous short courses and workshops on AQUATOX have been conducted by the development team over the years. The material has undergone extensive review and is provided for downloading from the [EPA AQUATOX Web site](#).

Several other versions and applications have been developed for other EPA offices and for other projects at OW. All these have been subject to QAPPs (Beach et al. 2000; Park 2002; AQUA TERRA Consultants and Eco Modeling, 2004; Park 2004; and AQUA TERRA Consultants and Eco Modeling, 2009, Horsley Witten, 2012); these QAPPs were used in the development and application of Release 3.1 plus.

In this project, AQUATOX Release 3.1 plus will be updated and updates will be documented under the requirements set forth in this QAPP. AQUATOX Release 3.2 is anticipated to be released following model update. The next section indicates the applicability of the QAPP in the context of the tasks.

A6. Project/Task Description and Schedule

The currently authorized phase of the work will involve the following primary tasks with QAPP applicability indicated:

1. The contractor shall develop a quality assurance project plan (QAPP). **(This document.)**
2. Improve representation of estuarine/coastal systems, consider automation of setup and explore enabling of linkages to hydrodynamics models and representation of complex water flows. **(Documentation, data migration, and model development.)**
3. Develop/implement indices within AQUATOX, which may include ecosystem indices similar to ECOPATH (e.g., production, consumption, connectance), and calibration statistics (e.g., Nash-Sutcliffe Model Efficiency Coefficient). **(Documentation and model development.)**
4. The contractor shall provide support for correcting errors in source code identified by the user community. The contractor shall also provide support for clarifying aspects of AQUATOX identified by the user as unclear. The EPA Principal Investigator will assign this task to the contractor on per issue basis. **(Pending assignment so QAPP requirements are unknown but should be covered by this QAPP.)**
5. The contractor shall develop new Graphical User Interface (GUI) and/or modify the existing GUI to generate and edit ASCII input file(s). The contractor shall also modify the source code such that the user should be able to run AQUATOX model without GUI by simply pointing to the ASCII input file(s). The contractor shall also modify AQUATOX source codes such that the model can produce ASCII output file(s). **(Documentation and model development.)**
6. AQUATOX currently stores data in a database management system (DBMS) called Paradox. Paradox is an obsolete DBMS with hard to find support. The contractor shall replace Paradox DBMS with a modern DBMS. EPA plans to use AQUATOX database for other modeling applications. The contractor shall build an API to access AQUATOX database. **(Documentation, data migration, and model development.)**

The schedule for completion, as shown in the Work Plan, is given in Table 2.

Table 2. Work Plan Schedule

DELIVERABLE	DATE DUE TO EPA
Task 1: Develop QAPP	Approval plus 2 weeks
Task 2: Improve Representation of estuarine/coastal systems	QAPP approval plus 10 weeks
Task 3: Develop/implement indices within AQUATOX	QAPP approval plus 15 weeks
Task 4: User support / refined documentation / error correction	Ongoing, as requested
Task 5: GUI development for ASCII input/output	QAPP approval plus 13 weeks
Task 6: Modernize DBMS and build API for updated database	QAPP approval plus 6 weeks

B. Secondary Data Acquisition and Quality Control

Only secondary data have been used in development of AQUATOX over the past 15 years. Wherever appropriate, we will insert a disclaimer in the Release 3.2 documentation stating “The quality of the secondary data has not been evaluated by the EPA for this specific application.”

Most tasks within the current work request involve model development, and do not involve secondary data acquisition. However, task 2 within this work request includes the migration of data developed within a non-EPA funded project (from the “nearshore marine environment” [NME] version of the model) into the EPA-released version of the model. This section will discuss secondary data requirements for quality control with respect to the migration of these new data sets.

B1. Sources of Secondary Data for this Work Request

As part of Task 2, parameters from the “AQUATOX Release 3.1 NME” version will be migrated into the EPA “AQUATOX Release 3.1 plus” database to create AQUATOX Release 3.2.

“AQUATOX Release 3.1 NME” was not created with EPA funding or subject to EPA quality assurance procedures. However, data for AQUATOX Release 3.1 NME has already gone through several levels of peer review. As part of the project that created these data, databases of model parameters were provided to scientists on the model-development team for review. Furthermore, AQUATOX Release 3.1 NME, and its parameter sets, underwent EPA-sponsored peer review in 2015 (Eastern Research Group, Inc. 2015).

Outside of Task 2, we do not anticipate that this work request requires us to collect additional data. If we are required to collect new secondary data for a specific task, this QAPP will need to be updated or a separate QAPP document will need to be prepared for the specific model application requested.

B2. Acceptance Criteria for Data

As part of Task 6 within this project (in which the AQUATOX databases will be updated to a modern DBMS), the CSRA team will build in a separate linked table pertaining to data source, data quality and suggested data usage that can be linked to each parameter (or group of related parameters). This will allow information about data quality to be incorporated into the AQUATOX database over time (if resources are available) and as new parameters are imported into the model.

There are two forms of data that will be imported into the AQUATOX 3.2 model domain (from AQUATOX Release 3.1 NME) as part of the current work request – 1. **Model Parameters** that are brought into the associated AQUATOX databases; and 2. **Observed or Driving Data** used in the calibration and verification of a specific model simulation.

1. **Model Parameters: AQUATOX** — like all food-web models, chemical fate and transport models, and bioaccumulation models — has dozens of parameters that need to be populated for the model to function properly. Some model parameters may be considered to be globally applicable (such as a chemical’s molecular weight), and others must be set on a site-specific basis (such as “periphyton critical force for scour,” which depends on a site’s substrate). Model parameters can be based on observed data, on literature studies, from other models, or from professional judgment and model calibration when other data sources are not available. In some cases, model parameters are not directly observable (e.g., allometric bioenergetics parameters) and need to be based on other calibrated models or professional judgment.

For this project, each model parameters for the calibrated estuarine models will be imported into the model and examined for data quality. In general, model parameters will not be rejected unless they are found to be errant. For example, a parameter would be rejected if it: falls outside of scientific plausibility (a negative number where there should not be), falls outside the range of a large body of observed data, or if a units error is encountered. If a model parameter is rejected, a new model parameter¹ will be used in its place and effects on model calibration will be noted and logged.

Each parameter imported into AQUATOX 3.2 will be examined by CSRA team staff and will have a note of its QA/QC status within the associated data-quality database (i.e., the date of QA/QC will be logged, the person doing the test, and the resulting “accept/reject”

¹ The new parameter will correct any units-conversion or “plausibility” error discovered. If the old parameter was rejected for falling outside the range of observed data, the new parameter it will be corrected such that it falls within the bounds of observed data and maintains the existing model calibration as best as possible.)

decision along with any accompanying notes). A separate log of each new parameter imported into the AQUATOX 3.2 databases will also be kept as part of this project.

2. **Observed or Driving Data:** Time-series observed data or time-series “driving data” are used in application-specific model calibrations and model verification. These data are generally both site specific and application specific and are therefore not saved as part of the distributed AQUATOX databases. However, these data are included in binary AQUATOX “APS” files, which archive all model input data, output data, and observed data used to assess model performance. As part of this work request, we propose that several sample APS files will be distributed with AQUATOX 3.2 that illustrate calibration to estuarine systems. These same files were submitted to the peer reviewers who examined AQUATOX Release 3.1 NME to demonstrate the model’s utility (Eastern Research Group, Inc. 2015). It is outside the scope of this work request to perform detailed quality review on all of the driving data and observed data used in these model applications. Instead, we will insert a disclaimer in the data-quality fields associated with the new data and also in the Release 3.2 documentation describing these model applications that states “The quality of the secondary data has not been evaluated by the EPA for this specific application.”

B3. System Documentation and Archiving

AQUATOX was one of the first environmental models to provide reference fields to document literature and other sources, conversions, and other information in the data input forms. These fields are provided in the model for the purposes of documentation and QA. A bibliography with full citations for the parameter values is available on the [EPA OST AQUATOX site](#) (U.S. Environmental Protection Agency, undated).

As discussed above, as part of this work request, our team proposes to build a linked table pertaining to data source, data quality and data usage that can be linked to each parameter in the AQUATOX database.

Extensive peer-reviewed documentation exists for AQUATOX. Any new documentation will be held to the same standards as was the documentation for Release 3.1 plus ([Park and Clough, 2014](#)), which is published on the EPA website. All model constructs are documented by providing the literature source, or as being original with AQUATOX.

Any manuscripts for publication in the open literature will be subjected to iterative editing involving WPC and other authors, and then reviewed internally by several EPA staff members and the EPA Principal Investigator. At this time no open-literature manuscripts are planned.

AQUATOX code changes and history are maintained using TortoiseSVN revision control / version control / source control software. Off-site backups of the code are made regularly. Multiple copies of source code and project documents will be kept for at least three years from the close of the project.

C. Model Development and Application

Development of new model enhancements is anticipated under Tasks 2-6. The procedures described below have been incorporated in previous QAPPs (Horsley Witten 2002) and used for prior EPA work assignments. If necessary, this QAPP will be amended when specific Task 4 assignments are determined; or a new QAPP specific to the application may be necessary. Since all of the requirements for this project are not known at this time, a general discussion of modeling requirements will follow.

This section will discuss model requirements for development and application with respect to: computer programming and tracking; the choice of model output; the process of model corroboration; and relevant acceptance criteria for model calibration and validation.

C1. Model Programming, Control, and Documentation

The variable names in the equations of the documentation correspond to those used in the program so that the mathematical formulations and code can be compared; the computer code is checked thoroughly for consistency with those formulations. All variables are documented in Appendix B of the Release 3.1 plus *Technical Documentation* (Park and Clough, April 2014). Existing AQUATOX coding conventions will be followed in any modifications of this software, and internal comments will continue to be used to allow for easier maintenance and future enhancement. During the development cycle the software will be run in the Delphi development environment, which alerts the programmer to problems with variable declarations and compiler errors. All changes to the code will be verified by a member of the team other than the programmer. Code changes will be posted on an EPA-available SVN revision control repository. The team-member reviewing the code change will document that he or she has reviewed each revision and keep a notice of the review and any suggested changes or refinements in a QA/QC code log for the project (Figure 2).

Testing, up to the beta version, is performed by the WPC programmer, another programmer on the WPC team, the CSRA unit tester, and the EPA Principal Investigator (at EPA's discretion). QA/QC will be tracked using an online cloud-based spreadsheet format (Google Sheets or similar) that is accessible to the whole team (Figure 2). This format should make transparent the status of the testing that was performed on each code update and the stage of the code for each task in the project.

WRR005 AQUATOX Code QA/QC Log ☆										
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A	B	C	D	E	F	G	H	I	J	K
	SVN Revision Number	Programmer Test Date	Programmer Comment #	WPC Test Completed	WPC Comment Number	CSRA Unit Test Completed	CSRA Comment #	Delivered to EPA	EPA Test (optional)	EPA Comment #
	217	10/1/2016	1	10/10/2016	2	11/1/2016	3	N/A	N/A	N/A
	218	11/6/2016		11/7/2016	4	11/9/2016	5	11/10/2016		
	Comment #	Comment								
	1	API to database completed								
	2	All code changes inspected, minor clarifying comments added, functionality tested								
	3	Suggested minor GUI changes for clarity								
	4	Minor GUI changes tested by WPC and code inspected								
	5	GUI changes satisfactory, ready for delivery to EPA								

Figure 2. Example of Code QA/QC log

Initial testing is performed by the programmer. It is the responsibility of the programmer to compile the source code for any new software component and exercise each function and code path within the new source code. All new code is tested in “debug mode,” which enables the programmer to view variables and their changing valuation as the code is executed on a line-by-line basis. The Delphi development environment provides strict typecasting and immediate feedback regarding compiler and run-time errors. Task 3 (the development of new output indices) includes code that will be tested with automated scripts using Delphi’s unit-test framework (DUnitX) based closely on Java (JUnit) and .Net (NUnit) testing frameworks.

Once all paths through the new code have been tested in the development environment, and using scripts when relevant, the alternative programmer is responsible for reviewing each line of the code and testing the enhancement under a suite of differing conditions. The alternative programmer will create test cases suitable for the scope of the enhancements under a variety of conditions. All EPA AQUATOX releases since Release 3.0 include rigorous mass balance tests to ensure that all inputs and outputs are included and balanced, and these tests are applied to each of the applications. Example studies will be compared with available field data.

Once a new version is ready for beta testing, the software installer is derived and tested on multiple computers and is then transmitted to CSRA and the EPA Principal Investigator for further testing. CSRA will verify that project requirements are met, that the model is well documented and user friendly, and ultimately that the model is acceptable. The model may also be made available to interested parties, primarily through the AQUATOX listserv. Feedback is generally provided by email and credible problems are acted on as soon as feasible, given Principal Investigator direction. Any required code changes are subject to the quality control procedures outlined within this document. All enhancements are commented in the code, including variable units. Logs are kept of programming changes, assumptions, and decisions made in model development and implementation; these, or pertinent excerpts, are submitted as deliverables in the project. Full source-code backups are regularly made and archived in a library that can be used to provide a snapshot of the full source code at various points of model

development. The TortoiseSVN SCM/source-control software for Microsoft Windows is used to track model revisions.

The *Technical Documentation* (Park and Clough April 2014) lays out the model equations with literature citations, or rationale if the construct is original. A master copy with Track Changes turned on is updated as changes are made and accepted. Units are provided to confirm the dimensional analysis. Mathematical formulations are programmed and graphed in spreadsheets and the results are evaluated in terms of behavior consistent with our understanding of ecosystem response. Much of this has been done as part of the continuing process of internal review. Releases 2 and 3 of the AQUATOX model and their documentation have undergone successful peer reviews by external panels convened by EPA, and a summary of the Release 3 peer review is on the AQUATOX Web site. Release 3.0 has also been described in the peer-reviewed literature (Park et al., 2008).

C2. Model Output for Calibration/Validation

If new model applications are assigned via Task 4, they will require calibration and possibly validation. AQUATOX produces voluminous quantities of output with varying availability and suitability of observed data for goodness of fit. Some of these data are straightforward and are most suitable for calibration and validation. Depending on the availability and uncertainty in observed data, and their direct vs. indirect applicability to AQUATOX predictions, others are less useful.

A general rundown of types of data that can be compared to AQUATOX outputs and a qualitative assessment of their usefulness in model calibration and validation are presented below:

- Concentrations of State Variables (***very useful because of data availability***)
 - organic matter, plants, invertebrates, fish
 - nutrients and dissolved oxygen, carbon dioxide
 - toxicants in water
 - concentration of toxicants within organisms
- Mass of Toxicants within State Variables, normalized to water volume (***less useful because these data are rarely available***)
 - T1-T20 in organic matter, plants, invertebrates, and fish

Others are calculated as secondary output based on simplifying assumptions. They are useful, but carry additional uncertainty:

- Additional Model Calculations (***very useful because of data availability***)
 - Secchi depth, chlorophyll *a*, TN, TP, BOD
- Biological Metrics (***less useful because they often represent short-term field studies***)
 - % of EPT, Chironomids, Amphipods, Blue-Greens, Diatoms, and Greens
 - Gross Primary Production, Turnover, Trophic State Indices

- Sediment Diagenesis State Variables such as nutrients in the sediments (*least useful because data are seldom collected with the spatial and temporal resolution of the simulation*)
- Toxicant Concentrations (*useful because of data availability*)
 - Concentrations in organic matter, plants, invertebrates, and fish
 - Bioconcentration Factors and Bioaccumulation Factors

Still others are useful for understanding the simulated mass balances and underlying processes that govern the model responses (*not used for goodness-of-fit*):

- Nitrogen and Phosphorus Mass Tracking Variables
- Uptake, Depuration
- State Variable Rates
- Limitations to Photosynthesis

The output also includes loadings (*not appropriate for goodness-of-fit*):

- Water volume, temperature, wind, light, pH

AQUATOX calibration tends to be an iterative process. The CSRA team will keep a detailed log tracking initial model parameters, their rationale, all parameter changes, and their effects on model outputs.

An AQUATOX simulation file (*.APS) contains all model inputs and parameters, external data used for model calibration, and all model outputs that were produced for the calibration run (including a library of saved plots). These files will be saved and archived along with the version of the model that was run to produce them and the calibration log file.

C3. Model Calibration and Validation

Model calibration is the systematic changing of initial model parameters to minimize error between observed and predicted values. The calibration process with AQUATOX is manual because of the model complexity. [A detailed example](#) is given in a technical note by Park et al. (2009a) and an abbreviated example along with additional guidance on calibration and validation is given in section 2.6 of the Release 3.1 plus [Technical Documentation](#) (Park and Clough, April 2014).

The validation process requires an evaluation of the model goodness-of-fit using an **independent** data set; that is, data that were not used in the calibration process. These data could be from another time period that is significantly different or from another water body.

C4. Acceptance Criteria for Calibration and Validation

It is not clear if any simulation development will be assigned under Task 4 of this work plan. If necessary, this QAPP will be amended when specific Task 4 assignments are determined; or a new QAPP specific to the requested model application may be necessary. For now, calibration and validation are discussed in general terms. AQUATOX simulations can be designed for a

variety of purposes, ranging from a teaching study, to a proof of concept, to a model application designed for evaluation of different policy options. The stringency requirements for calibration may vary considerably depending on the intent of the model-application developer.

The requirement for model concordance with data also depends on the quality of the calibration data sets. There are often uncertainties in biotic data (or even lack of data) in contrast to general water quality data. For example, target endpoints may be periphytic chlorophyll *a* (measured on cobbles a couple of times a year), biomass of sestonic blue-greens (perhaps measured biweekly in the growing season), or biomass of largemouth bass (with observed data being *numbers* of bass captured by electrofishing in a poorly defined reach). Sporadic observed data make it especially difficult to perform pair-wise comparisons of simulated and observed values.

Therefore, we usually apply a weight-of-evidence approach with a hierarchy of tests emphasizing discernment of similar simulated and observed patterns:

- Reasonable behavior based on general experience;
- Visual inspection of data points and model plots (weight of evidence approach);
- Inspect if model predictions fall within error bands of data;
- Inspect if point observations fall within model bounds obtained through uncertainty analysis;
- Check concordance and bias using regression of paired data and model results;
- Comparison of mean data and mean model results; and
- Comparison of frequency distributions, such as Relative bias (Bartell et al., 1992), F test (comparing the variance of predicted and observed data sets as used in Park et al. 2009a, and taken from Bartell et al., 1992), and Kolmogorov-Smirnov test (Sokol and Rohlf, 1981).

Model fit should be evaluated using different time periods depending on the system. Short-term processes may be evaluated by daily comparisons while seasonal bias can be evaluated using monthly comparisons. Long-term effects, such as recovery from a significant toxicant spill, can be evaluated using yearly or overall comparisons. Guidance for evaluating model fit acceptance criteria is given in Table 3.

Table 3. Metrics for Evaluating Model Fit with Suggested Acceptance Criteria

Metric for Model Fit	Acceptance Criteria	
	Good	Fair
Reasonable behavior	Stable seasonal fluctuations	Unexplained deviations from stability
Visual comparison output and observed data	Concordance, few outliers	Concordance, multiple outliers
Predictions within data error bands	± 1 std dev	± 2 std dev
Point observations within model bounds	± 1 std dev	± 2 std dev
Percent difference in means*	15 to 25%	25 to 35%
Relative bias (means)	0 ± 1 std dev	0 ± 2 std dev
F test (variances)	0.67 to 1.5	0.33 to 3.0
Kolmogorov-Smirnov test	< 0.05 p value	< 0.1 p value

* for select variables, depending on modeling goal

D. Project Assessment and Oversight

D1. User Evaluation and Reconciliation

Quality objectives are addressed in this QAPP for both data acquisition (Section B) and modeling development and application (Section C). Acceptance criteria for data and model calibration were selected to ensure achievement of the quality objectives. If there are irreconcilable discrepancies from the quality criteria, the ability of the model to achieve quality objectives and provide accurate output might be compromised. Under such circumstances, the consultant will confer with EPA to determine if the quality discrepancies could still allow user requirements to be met. If not, then a plan to address the issue will be developed to ensure model quality and user satisfaction.

D2. Agency Evaluation and Reporting

Monthly progress reports will be submitted to the EPA Principal Investigator. These progress reports will include a detailed breakdown of costs and hours, a description of activities and QA by task, a discussion of any problems encountered, and percent completion of the project.

Because Task 4 is not completely specified, there will be several possible deliverables, each providing EPA with opportunity either to approve products and decisions or to request changes:

- Quality assurance project plan (QAPP);
- Documentation of AQUATOX enhancements;
- Study files and calibration logs for applications;
- Technical guidance materials; and

- Oral presentation material.

The response of EPA staff to these products will provide additional external quality control.

E. Literature Cited

- AQUA TERRA Consultants and Eco Modeling. 2004. Quality Assurance Project Plan: Technical Support Activities for AQUATOX. U.S. Environmental Protection Agency, Washington, DC.
- AQUA TERRA Consultants and Eco Modeling. 2009. Quality Assurance Project Plan: EP-C-06-029, Work Assignment 3-11, Amendment 1 U.S. Environmental Protection Agency, Washington DC.
- Bartell, S. M., R. H. Gardner, and R. V. O'Neill. 1992. Ecological Risk Estimation. Lewis Publishers, Boca Raton, Florida.
- Beach, R. B., J. S. Clough, P. M. Craig, A. S. Donigian, R. A. McGrath, R. A. Park, A. Stoddard, S. C. Svirsky, and C. M. Wallen. 2000. Quality Assurance Project Plan: Modeling Study of PCB Contamination in the Housatonic River. GE-100500-AADY, U.S. Army Corps of Engineers, Concord Mass.
- Clough, J. S. 2014. AQUATOX (Release 3.1 plus) Volume 1: User's Manual. EPA-820-R-14-005, U.S. Environmental Protection Agency, Washington D.C.
<https://www.epa.gov/sites/production/files/2014-03/documents/user-s-manual-3-1.pdf>.
- Eastern Research Group, Inc. 2015. "Peer Review of EPA's AQUATOX Release 3.1 with Nearshore Marine Environment Modifications. Task Order 50 Under Contract EP-C-12-029." Final. September 1, 2015.
- Horsley Witten Group, Inc., and Warren Pinnacle Consulting, Inc. (2012). "Contract EP-C-12-006. Quality Assurance Project Plan for Work Assignment No. B-01. Technical Support Activities for AQUATOX."
- Park, R. A. 2002. Quality Assurance Project Plan: Development of an Estuarine Model of AQUATOX and Analysis of Perfluoroalkylated Surfactants. EPA Contract 68-C-98-010, U.S. Environmental Protection Agency, Washington DC.
- Park, R. A. 2004. Quality Assurance Project Plan: Atrazine Modeling with AQUATOX. EPA Contract 68-C-98-010, WA 2-04, U.S. Environmental Protection Agency, Washington DC.
- Park, R. A., J. N. Carleton, J. S. Clough, and M. C. Wellman. 2009a. AQUATOX Technical Note 1: A Calibrated Parameter Set for Simulation of Algae in Shallow Rivers. EPA-823-R-09-003, U.S. Environmental Protection Agency, Washington D.C.
https://www.epa.gov/sites/production/files/2014-03/documents/2009_02_09_models_aquatox_technical_technote01.pdf

- Park, R. A. and J. S. Clough. 2009b. AQUATOX (Release 3) Volume 2: Technical Documentation. EPA-823-R-09-004, U.S. Environmental Protection Agency, Washington D.C.
- Park, R. A. and J. S. Clough. 2012. AQUATOX (Release 3.1) Volume 2: Technical Documentation. EPA-823-R-09-004, U.S. Environmental Protection Agency, Washington D.C.
http://warrenpinnacle.com/prof/AQUATOX/AQUATOX_Release_3.1_Technical_Documentation.pdf
- Park, R. A. and J. S. Clough. 2014. AQUATOX (Release 3.1 plus) Volume 2: Technical Documentation. EPA-820-R-14-007, U.S. Environmental Protection Agency, Washington D.C. <https://www.epa.gov/sites/production/files/2014-03/documents/technical-documentation-3-1.pdf>
- Park, R. A., J. S. Clough, and M. C. Wellman. 2008. AQUATOX: Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems. *Ecological Modelling* **213**:1-15.
- Sokol, R. R. and F. J. Rohlf. 1981. *Biometry: The Principles and Practice of Statistics in Biological Research*. Second edition. W.H. Freeman and Co, San Francisco.
- U.S. Environmental Protection Agency. Undated. Bibliography for AQUATOX Libraries. <https://www.epa.gov/sites/production/files/2014-03/documents/aquatox-data-libraries.pdf>.
- U.S. Environmental Protection Agency. 1999. QAPP Requirements for Secondary Data Research Projects: Example Guidance by the QA Managers in EPA's National Risk Management Research Laboratory.
- U.S. Environmental Protection Agency. 2002. Guidance for Quality Assurance Project Plans, EPA QA/G-5, EPA/240/R-02/009. <https://www.epa.gov/quality/guidance-quality-assurance-project-plans-epa-qag-5>.
- U.S. Environmental Protection Agency. 2002. Guidance for Quality Assurance Project Plans for Modeling, EPA QA/G-5M, EPA/240/R-02/007. <https://www.epa.gov/quality/guidance-quality-assurance-project-plans-modeling-epa-qag-5m>.