Executive Summary

Peer Review of *"AQUATOX (Release 2 Beta Version)"*

Prepared for:

U. S. Environmental Protection Agency
Office of Water
Office of Science and Technology
Standards and Health Protection Division
1200 Pennsylvania Avenue, NW
Washington DC 20460

Prepared by:

Tetra Tech, Inc.
10306 Eaton Place, Suite 340
Fairfax, VA 22030

March 2003

EXECUTIVE SUMMARY

Background

AQUATOX is a personal computer-based ecosystem model that simulates the transfer of biomass and chemicals from one compartment of an ecosystem to another. EPA is currently developing Release 2 of the model, which has important additions to previous versions, including development of a "Wizard" that guides the user through the model setup process; enhanced graphing abilities; increased number of biotic compartments and organic toxicants that can be simulated in a single run; and an extension to BASINS (Version 3.0) to enable *AQUATOX* to take advantage of data layers, watershed loading models, and postprocessing capabilities of BASINS. EPA contracted with Tetra Tech, Inc. to perform a peer review of *AQUATOX* Release 2. Tetra Tech used three expert consultants (Don DeAngelis, Ecologist, U. S. Geological Survey, Biological Resources Division and Adjunct Professor, Department of Biology, University of Miami; Rob Pastorok, Senior Editor, Ecological Risk Assessment for *Human and Ecological Risk Assessment*; and Frieda Taub, Professor Emeritus, School of Aquatic and Fishery Sciences, College of Ocean and Fisheries Sciences, University of Washington) to review the beta version of *AQUATOX* Release 2 and make recommendations. The peer review focused on the strengths and weaknesses of *AQUATOX* Release 2 (beta) from a scientific and regulatory perspective. A summary of the peer review is provided below.

General Findings

The peer reviewers found *AQUATOX* to be a useful tool for determining a variety of effects on aquatic ecosystems:

> *I am very impressed with AQUATOX as a tool for use in various types of assessments of toxicant and other stressor impacts on aquatic ecosystems.*
>
> *AQUATOX is a valuable tool for analyzing environmental issues related to aquatic ecosystems.*
>
> *AQUATOX is a useful and insightful model for exploring the likely fate and effects of toxic chemicals on a variety of aquatic ecosystems, using our current level of understanding about ecological relationships.*

All of the peer reviewers recommended that AQUATOX is ready for release after making some minor suggested modifications, mostly to the technical documentation.

Is *AQUATOX* Scientifically Sound?

The peer reviewers found the *AQUATOX* ecosystem model and its components were scientifically sound and that the technical documentation for the model was consistent with findings in current ecological literature. The underlying assumptions used in *AQUATOX* were found to be based on tested scientific model formulations of ecological processes and were

backed up by appropriate references to scientific publications. *AQUATOX* also allows the user to rely on professional judgment to modify assumptions and inputs where necessary. The reviewers agreed that *AQUATOX* had been adequately verified for a variety of water body types for estimation of water quality (e.g., nutrient and dissolved oxygen concentrations) and lower trophic level responses (e.g., algal and periphyton growth).

The reviewers determined that mathematical formulations used in the components of *AQUATOX* were appropriate and accurately reflect the ecological processes they are intended to simulate. The reviewers agreed that *AQUATOX* was useful for predicting a variety of ecosystem effects resulting from a variety of stressors such as nutrients, toxics, and organics. They concluded that the simplifying assumptions in the model were reasonable but users of the model will need to determine which of the parameters should be used or modified for a particular site.

Is *AQUATOX* Reasonable in Its Predictions?

Overall, the reviewers agreed that the predictions from *AQUATOX* were reasonable and adequately reflected ecological processes and behavior. They also found that the ability of *AQUATOX* to model processes for biological guilds in several trophic levels and associated feedbacks was excellent. The reviewers noted that *AQUATOX* should not be generally used to make accurate predictions about specific changes in variables, especially for indirect effects, because studies on the direction and magnitude of change for most of these variables in response to stressors have not been published yet. However, when site specific studies are desired, using *AQUATOX* with data collected at the site for calibration and validation of the model can be an appropriate application.

The reviewers commented that *AQUATOX*, like all models, makes simplifying assumptions and could be vulnerable to challenge if a regulated party objects to the outcome. For site-specific predictions, a great deal of calibration and alterations in the level of the model's complexity might be required before it can be used. Estimates of toxicity in the model are based on a few, well tested species, which might not be representative of the toxicity that would be experienced by site-specific biota. The reviewers were uncertain about the chronic effects results predicted by *AQUATOX* because the model uses acute effects data to predict many chronic effects.

The reviewers noted that *AQUATOX* can be used to support empirical assessments to determine which stressor is causing an impairment, and AQUATOX may be useful for evaluating some causal relationships. The reviewers agreed that increasing the calibration and parameterization of *AQUATOX* would increase the accuracy of the model's predictions.

Is *AQUATOX* Usable?

The reviewers agreed that *AQUATOX* appeared to be comprehensive and it sufficiently represented the structure of complex aquatic ecosystems that were homogeneous along the horizontal dimension. They found that *AQUATOX* was flexible enough to predict effects of perturbations on various kinds of food webs with a wide range of complexities. They also thought that the flexibility of the model would support the modeling of a variety of waterbody types and stressor types, and various applications from general to site-specific. Also, the model should be capable of modeling the fate of compounds with robust data sets as well as sparse data sets, although assessments using sparse data sets should be qualified.

The reviewers agreed that the model could be used to highlight possible relationships between stressors and various ecological outcomes. AQUATOX was also found to be useful for evaluating the sensitivity of response variables to various stressors with varying degrees of uncertainty. They agreed that the ability to run "Control versus Perturbed" ecosystem evaluations was useful for comparative or screening analyses.

The reviewers found that the data libraries of *AQUATOX* were very useful and well developed. They agreed that the user interface was user-friendly and that the *AQUATOX* Wizard was helpful. The reviewers also liked several other *AQUATOX* features, including the uncertainty analysis, which allowed output to be produced in tabular and graphic forms; the Control Setup, which was easy to use and made parameterization of control simulations easy; and the ability to add or delete state variables (interrelated components in aquatic ecosystems), which is useful because not all state variables exist at all sites.

Is *AQUATOX* a Credible Tool for Various EPA Programs?

The reviewers agreed that *AQUATOX* is a credible, powerful, quantitative tool for regulatory decisions if the results are used appropriately and if it is one of several sources of information used to make a regulatory decision. Results from *AQUATOX* can be used as an information input to decisions concerning particular ecological stressors.

The reviewers agreed that with appropriate calibration and testing for specific applications, *AQUATOX* could be used in many EPA programs, including RCRA risk assessments, TSCA evaluations, and pesticide registration decisions. Because *AQUATOX* does not model the effects of metals, there is a gap in the utility of the model for site-specific assessments under Superfund, RCRA, or state cleanup programs where mixtures of metals and organic compounds are present. The model can be used to screen chemicals to determine the need for toxicity tests or other tests. *AQUATOX* might be useful in determining the outcome of impacts from setting criteria at specific levels. The model also can be used to analyze alternative pollution control scenarios and restoration strategies.

The reviewers found that the model could be used to evaluate the implications of setting TMDLs within a specific range and to evaluate the effects of load reductions. They determined that it may be difficult to use the current version of *AQUATOX* to develop some TMDLs. For example,

in some eutrophication TMDLs since AQUATOX does not maintain a strict mass balance of nutrients, the model results might only be useful for evaluating relative impacts of nutrient inputs on the waterbody.

Summary of Recommendations

Overall, the reviewers suggested that more model validation and calibration be performed using additional systems from published literature, particularly calibration of the bioaccumulation and bioconcentration functions of the model. *AQUATOX* could be enhanced to include program- and use-specific validation criteria for particular applications based on the level of accuracy required. Also, measures of parameter variability (e.g., range and standard deviation) could be used in the validation process and added to the data libraries. The reviewers suggested that model validations be published in peer-reviewed literature, especially for toxicant effects on biota. They also suggested that more guidance be added to the technical documentation to illustrate how users can appropriately calibrate the model based on the intended use of the results.

The reviewers agreed that enhancements could be added to *AQUATOX* for determining the effects of perturbations on food webs. For example, food web diagrams (with lines of varying thicknesses denoting the magnitude of the relationships between categories) might enable the user to identify keystone species, determine interaction strength for each species, and measure biological community stability. The reviewers suggested that the model developers review the model components related to trophic levels in the food web to determine the accuracy of this feature.

The reviewers suggested that the user's manual should be updated for the current version of *AQUATOX*. They suggested that the *AQUATOX* technical documentation and user manual could be enhanced, including an explanation of model output units, batch mode operation and setup, and concepts such as using bioaccumulation factors and bioconcentration factors used to constrain model calculations. Additional sections including information on uncertainty and technical definitions would also enhance the technical documentation. The technical documentation should include a list of processes and fluxes that are approximated or not included in the nutrient mass balance. The user's manual should also mention how automatic scaling of graphical outputs may obscure changes to parameters of interest. The reviewers suggested that the model documentation incorporate a more detailed explanation, including references to supporting documents, of algal and fish biomass and PCB bioaccumulation predictions.

The reviewers suggested that the relationship of external chemical concentrations to physiological effects via internal chemical concentration should be validated for more chemicals in future versions of *AQUATOX*. The number of species used for toxicity estimates could be increased to reduce the uncertainty of the model's results. Also, additional sensitivity analyses of the toxicity estimates would help to determine how over- or under-estimates of toxicity will affect the model results.

The reviewers agreed that future versions of *AQUATOX* should include more detail about decomposers, so the model can be used to determine a toxicant's effects on these organisms. The representation of the detrital food web in *AQUATOX* could be clarified in the technical documentation. Also, later versions of *AQUATOX* should move toward a more complete mass balance of key nutrients.

The reviewers suggested that additional capabilities could be added to *AQUATOX* including the ability to model metals, to model more than two sediment feeders at once, and to allow the user to choose different types of functional responses for consumption. In addition, they suggested that the ability of *AQUATOX* to model rivers and spatially heterogeneous lakes and reservoirs would be improved in future versions by allowing segmentation, horizontal heterogeneity, and vertical disaggregation of streams into zones of free-flowing water and bottom boundary layers. Other suggested improvements included adding a summarized setup to the program to let other users know immediately whether a state variable has been eliminated; simplifying the model for specific applications or on a site-specific basis; including effects of wave agitation on macrophytes; adding an "optimal control" feature that allows TMDLs to be calculated based on a prescribed set of criteria; and improving the Monte Carlo tool portion of *AQUATOX* so that it addresses the treatment of correlations among variables.

One of the reviewers suggested that a future version of *AQUATOX* be developed for use in teaching ecosystem ecology courses. It should include features such as the microbial loop, the decomposer food chain, rigorous mass balance, and complexing of nutrients in sediments with ferric ions and calcium.