



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON D.C. 20460

OFFICE OF
WATER

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MEMORANDUM

SUBJECT: Peer Review of AQUATOX Release 2

FROM: Peter Grevatt, Acting Director, Standards and Health Protection Division (4305T)
Office of Science and Technology, Office of Water

Oscar Hernandez, Director, Risk Assessment Division (7403M),
Office of Pollution Prevention and Toxics

TO: Peer Review File

BACKGROUND

AQUATOX is a simulation model for aquatic ecosystems. It was first released in September 2000, and development has continued since that time. Release 2 of AQUATOX improves both the ecological and analytical functions of the model, and the usability of the model in terms of data acquisition and the user interface. Prior to making AQUATOX final and available to the public, the beta version and draft documentation underwent external peer review.

The peer review took place during the summer and fall of 2002. It was done under contract to Tetra Tech, Inc. (contract # 68-C-01-022). The peer review panel consisted of three independent reviewers. The format was a series of facilitated conference calls and subsequent submission of written comments.

The objectives of the peer review were to:

- Review the conceptual design of *AQUATOX* Release 2 and evaluate whether the model is consistent with published ecological literature.
- Evaluate whether sufficient and appropriate ecological processes are included to represent the combined fate and effects of organic toxicants, nutrients, and other stressors.

- Evaluate the reasonableness of *AQUATOX* predictions.
- Determine the overall utility of the model including: user-friendliness, data needs, and interface capabilities. Review the *AQUATOX* Release 2 documentation for clarity, ease of use, and scientific veracity and suggest improvements where necessary.
- Evaluate whether *AQUATOX* Release 2 (beta) provides a sound and credible tool to the EPA Headquarters, regions, states, and local governments for ecological risk assessments of toxic chemicals, and for water management programs, including assessment of water quality criteria, and TMDL development.

The attached Record, prepared by Tetra Tech, contains the complete charge to the panel, the names, affiliations and Curriculum Vitae of the panel members, summaries of the conference calls, summary report on the panel findings, and other materials.

GENERAL PANEL FINDINGS AND RECOMMENDATIONS

The overall review was highly favorable, and the panel recommended that *AQUATOX* Release 2 is ready for release to the public and for application in a variety of ways, after some editing to the technical documentation and user's manual. The following quotes are taken from the Executive Summary:

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.

The panel agreed that the model is scientifically sound, and consistent with current ecological literature. They determined that the ecological processes are accurately simulated, the simplifying assumptions included are reasonable, and that model predictions were reasonable. The mathematical constructs and simplifying assumptions are well documented.

With regard to model application, they noted that individual processes may not be detailed enough in certain situations, depending on the complexity of the ecosystem and the type analysis required. Specific applications may require additional enhancements, or extensive calibration to sufficiently characterize the existing conditions. The panel pointed out that the model output, as with many complex models, could be subject to dispute if they disagree with the outcome. Thus sufficient and explicit documentation of model constructs and assumptions is essential.

One area of concern regarded nutrient analysis. AQUATOX does not maintain a strict mass balance of nutrients as it does for toxicants and most other state variables. Specifically, the model allows release of nutrients into the water column by rooted macrophytes, but they do not explicitly take up nutrients from the sediment pore water. There are also some nutrient processes that are not included in the model, namely, complexation of phosphorus with sediments and its release under anaerobic conditions. Some expressed concern that, for those situations where excluded processes are significant, a comprehensive eutrophication analysis that requires a strict mass balance might not be possible. If the excluded processes are not a significant factor in the system, there would not be a problem. However, the reviewer went on to say that even where the excluded processes are important, using the model to compare relative differences between various management scenarios would be a valid application of AQUATOX.

The panel considered AQUATOX to be substantially verified, and validated for several types of endpoints. However, additional validation would increase user confidence and lend greater credibility to its use. The specific area recommended for additional validation was biological effects from toxicants. However they also noted that complete validation, in the sense of comparing model predictions with observed data, for all endpoints predicted by AQUATOX is probably not feasible, especially where there is a complex biological community, higher trophic levels, indirect effects or multiple stressors. Data to support that kind of validation exercise are probably not available at this time.

The panel found the model to be user friendly. It is also very flexible, enabling users to tailor it to their ecosystem and analytical needs. Therefore it is applicable to many types of environmental analyses in a variety of contexts, including in support of ecological risk assessments for RCRA and TSCA, pesticide registration decisions, stressor identification, TMDLs, water quality criteria and standards, and analyzing pollution control management alternatives.

The panel was unanimous in recommending that the model was ready for release, following some editing of the technical documentation and user's manual.

PANEL RECOMMENDATIONS and OST RESPONSES:

Documentation: The peer reviewers offered specific recommendations for edits to the documentation, including laying out more explicitly the model's simplifying assumptions and more clearly articulating which ecological processes are and are not included. They also recommended expansion and clarification of certain sections, including the descriptions of the uncertainty analysis and the toxicology constructs. In addition, the User's Manual and its graphics need to be updated to reflect the new interface and new capabilities, and the included tutorial expanded.

We are in the process of making the edits and improvements to the technical documentation and user's manual as recommended by the panel.

Appropriate model application: The panel recommended that EPA make clear the appropriate usage of AQUATOX and complex models in general, in any training or guidance materials. In particular, they cautioned that very precise predictions for higher trophic levels effects, indirect effects, specific processes, and multiple stressors was probably not a realistic expectation, at least not without extensive efforts to parameterize and calibrate the model to the site and resident ecosystem. However reasonable estimates can be obtained, along with estimates of uncertainty.

This comment is germane to many models, in that all are representations of reality, not reality itself. Therefore no model can provide proof of anything, however it can be used as a tool to help provide realistic projections of future conditions and/or plausible explanations of observed conditions. This is particularly true for complex models such as AQUATOX. Projections that are a result of indirect effects are even more problematic, as they are extremely difficult to validate with independent data. The particular reviewer making this comment went on to say, however, that estimates can be made with AQUATOX, along with providing measures of uncertainty and confidence limits around the predictions. In training and/or outreach materials we will attempt to accurately convey what models (including AQUATOX) can and cannot do.

Model Validation: The panel recommended that EPA undertake more model validation, particularly for biotic effects and higher trophic level effects of toxicants. They noted that although there had been one 1998 validation report prepared for OPPT using mesocosm data, confidence in the biotic effects (especially higher trophic level fish) portion of AQUATOX could be strengthened by examining additional data sets, and suggested several sources of data. They did not recommend that this had to be done before Release 2 was made public, however. One reviewer also recommended that additional validation be done on the method the model uses to convert external water concentrations to internal (body) levels and consequent physiological effects. (She did however commend this method as being very innovative and a scientifically sound approach.) The panel also made several suggestions about developing some form of validation criteria.

We agree that more validation is always better, in order to build confidence in and experience with the model. This task has been included in the new work assignment, although the details have not been worked out. The specific endpoints and particular chemicals or types of chemical tested will depend on resources and data availability.

Uncertainty analysis: The panel liked the uncertainty analysis feature and recommended its use for sensitivity analysis and for determining site specific data needs. They recommended that future versions add the ability to include estimates of correlation between variables, which are now assumed to be dependent.

We are investigating the incorporation of correlations among variables into the uncertainty analysis utility. Depending upon the complexity of the task and effort required, it may be added. It could be a valuable option for those cases where there are significant correlations between variables at a site, although it is not clear how often this capability would add significantly to an analysis. However it must be recognized that it is unlikely that most users would have the

information available to quantify the correlation among variables.

Nutrients: One reviewer recommended that we attempt to add more nutrient processes in order to get a closer approximation of full mass balance for nutrients. Although he noted that it was not necessary, nor even possible to develop a complete characterization of all nutrient fluxes, as some processes are not fully understood, he recommended getting as close as possible. He went on to say that even where mass balance is not complete, AQUATOX could still be very useful in a relative sense, particularly in examining relative effects of management alternatives on a waterbody.

We agree that a more strict mass balance of nutrients would improve the ability of AQUATOX to model those sites where the currently excluded processes are a significant portion of the nutrient dynamic, and improve confidence in the model. It would not be a trivial undertaking, however, as it would require the inclusion of explicit nutrient uptake by macrophytes, pore water nutrient concentrations, complexation of phosphorus with sediments and its release under anaerobic conditions, and time varying pH.

Data: There were several suggestions dealing with improving input data. AQUATOX includes tools to estimate toxicity data in the absence of species data, and although they did not disagree with this tool, they cautioned that the absence of species-specific data could add a source of contention, and uncertainty to a model application. Therefore they recommended expanding the default data sets to as many species, and for as many chemicals as possible. A related recommendation was to include some measure of variability to the default parameter sets. They also agreed that BASINS linkage was a good addition as a means of acquiring site and loading data

We agree that the better the data input, the better the output. We have provided much default data, however in all cases the user can substitute current or specific data. We will attempt to expand the default data set as much as possible; at a minimum, it will grow as the developers model more species and get better calibrations for existing sets. With regard to the estimation of toxicity parameters from a small number of species, we agree that the estimation of parameters is less preferable than actual data. However, we recognize that is not always possible, so we have provided these features so the user can make work in data poor environments but make reasonable estimate. There is ongoing work within the Agency at the Gulf Ecology lab to improve the regression equations to estimate toxicity between species. If possible and appropriate, we will take advantage of that work to improve the estimations within AQUATOX.

Future development: The panel made numerous other recommendations for future enhancements and refinements. The most significant in terms of effort are:

- develop the ability to simulate metals
- increase the options for spatial segmentation, for both finer spatial resolution (vertical and horizontal), and larger scale (linked segments)
- add an option for a hourly time step

- develop additional tools for ecosystem analysis, such as diagrams of food webs, evaluation of species interactions and keystone species
- increase the complexity of how detrital food web and decomposition (organic sediments) are simulated
- simplify the model for specific applications

All of these will require further examination and consideration, and the decision whether to undertake them will be dependent upon resources, and the value added for the primary users of the model.

There have been a few changes to Release 2 since the time of the peer review conference calls. Primarily they are enhancements that were in progress at that time, and which the panel was advised of. Panel reaction to these additions was favorable, although they did not actually test them. The primary changes are:

- completion of the habitat disaggregation for streams to allow habitat preferences for the biota
- completion of the testing and linkage of inorganic sediments from HSPF as part of the BASINS extension
- completion of bryophytes (mosses) as an additional biotic compartment
- correction of an error related to bioenergetics that had originated from the Wisconsin Bioenergetics Model

Although not part of Release 2, the estuarine version of AQUATOX for the ecological evaluation of perfluorinated organics for OPPT has also been completed.

For more detail on the specific recommendations from the panel and our responses found in the Attachment, Peer Review Comments and EPA Responses. The full text of written comments and recommendations can be found in the attached report, "Record for the Peer Review of AQUATOX Release 2 (beta version)".

Attachments