MEMORANDUM

Date: JUL 21 2009

Subject: External Peer Review to AQUATOX Release 3

From: Denise Keehner, Director
Standards and Health Protection

To: Peer Review file

BACKGROUND

AQUATOX is an ecosystem model for aquatic systems. It predicts the fate of various pollutants and their effects on the ecosystem. EPA issued AQUATOX Release 1 in 2000. Since then, the model has been improved and released several times. EPA is currently beta testing AQUATOX Release 3, which is the subject of this expert peer review.

In summer 2008, Eastern Research Group, Inc. (ERG), an EPA contractor, organized an independent teleconference peer review of AQUATOX Release 3 to help EPA enhance the quality and credibility of the AQUATOX Release 3 model. Because Release 2 of AQUATOX had already been externally peer-reviewed, this review primarily focused on the many enhancements made to the model since Release 2. A list of the enhancements is provided in the Charge to Reviewers in the attached Peer Review Report.

The peer reviewers were asked to respond to a number of charge questions concerning the following objectives:

- Review the scientific basis of *AQUATOX* and evaluate whether the model is consistent with published ecological literature. Particular attention should be paid to the enhancements made since the Release 2 peer review.
- 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.

- Evaluate whether *AQUATOX* Release 3 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 quality management programs, including development and assessment of water quality criteria, biocriteria, refinement of designated uses, and total maximum daily load (TMDL) development.
- Determine the overall utility of the model: user-friendliness, data needs, and interface capabilities.
- Review the user documentation for clarity, ease of use, and scientific veracity and suggest improvements where necessary.

The complete charge questions are provided in the Charge to Reviewers (attached).

GENERAL PANEL FINDINGS AND RECOMMENDATIONS

The reviewers were in unanimous agreement that AQUATOX Release 3 represents a significant improvement over previous versions, and that the enhancements to the model are substantial. The reviewers specifically commented that the enhancements improved the model's utility and flexibility. They thought that the enhancements to the uncertainty and sensitivity analyses were among the most powerful additions to the model. They also commented that the simplifying assumptions were transparent, helpful, and necessary. All reviewers found the default values provided by AQUATOX to be well documented and scientifically acceptable. They thought the ability to replace the default values with other values was easy, innovative, and useful.

While the reviewers agreed that the enhancements to the model were scientifically sound, one reviewer pointed out that it is not possible for the model to be consistent with *all* positions expressed within the scientific literature because consistency within the literature does not exist. Two reviewers said it was hard to measure the model's reasonableness, arguing that its reasonableness depends on its end use, and it is up to the user to determine the appropriateness (i.e., "reasonableness") of the model's simplifying assumptions.

While the reviewers generally agreed that the predictions of the model appear to accurately reflect currently accepted ecological processes and behavior, they cautioned that a complex model such as AQUATOX cannot be expected to provide high precision. They stressed the importance of documenting the model's calibration and validation, and recommended that additional information about the model's calibration and validation be presented. One reviewer suggested creating an AQUATOX Case Study document to more fully document the calibration and verification studies that have been done to date. The reviewers agreed that AQUATOX could be applicable to a variety of water body types; however, they stressed that each one would have to be calibrated and validated for meaningful conclusions to be drawn.

All reviewers agreed that the model is sufficiently flexible to accommodate a variety of applications. The reviewers commented that analyzing pollution control scenarios was one of the most exciting applications of the model. Other suitable applications for AQUATOX, especially if sufficiently calibrated and validated, were ecological risk assessments, and Total Maximum Daily Load analysis and development. Other applications were more appropriate if done in conjunction with other tools and approaches, in a weight of evidence approach for example. These applications included identification of potential stressors causing

impairment of aquatic life, evaluation of causal relationships between chemical and physical stressors and their combined effects on aquatic biota, and supporting the existing approaches used to develop water quality standards and criteria.

The reviewers agreed that the latest enhancements to the AQUATOX model improved the suitability of the model's application to federal and state government decision-making. One reviewer commented that the "model enhancements have made AQUATOX one of the most exciting tools in aquatic ecosystem management." Another said that "this is the first model that provides a reasonable interface for scientists to explore ecosystem level effects from multiple stressors over time." However, all reviewers again stressed the importance of model calibration and validation for site-specific decision-making.

All reviewers agreed that the enhancements made to the Graphical Users Interface and output variables of the AQUATOX model (including the Wizard, unit conversions, integrated users manual, and context-sensitive help files) were invaluable and vastly improved the model's overall utility. Specifically mentioned were the sensitivity analysis and tornado diagrams and the inclusion of EPA's Office of Research and Development's Interspecies Correlation Estimates (ICEs) database and statistics. One reviewer commented that as long as the uncertainties are quantified, "the integration of ICE data into AQUATOX makes this model one of the most comprehensive aquatic ecotoxicology programs available."

Likewise, the reviewers thought the Technical Documentation was well-written, thorough, and accurate. They offered several suggestions for expansion or clarification of text. To supplement the Technical Documentation and User's Manual, one reviewer recommended that an "AQUATOX Case Study" document could also help the user to appropriately apply the model to complex situations.

Now that the model is so user-friendly and accessible, two of the reviewers expressed concern that less skilled modelers could misuse the model or use AQUATOX in a "plug and chug" fashion. To avoid this, the reviewers felt strongly that a "mission statement" addressing the intended use of the model be added to the documentation. One reviewer specifically recommended a "user beware" sentence which states that "AQUATOX should only be used (beyond screening purposes) in instances where it can be sufficiently calibrated and validated on a site-specific basis," and that "it is the responsibility of the user to carefully consider the default values and judge the appropriateness of the values relative to the specific application for which the model is being used." The reviewers also stressed the need for having adequate support available to assist users with model setup and application.

The reviewers agreed that the AQUATOX model is adequately complex and did not recommend that additional ecological processes be added to this version. They acknowledged that substantial improvements have been made to the model, the user interface, and the supporting documentation. They agreed that future efforts should focus on model calibration and validation, as well as more explicit documentation where needed.

The reviewers did offer some suggestions for future model enhancements, though none were necessary for inclusion into Release 3. The most significant new scientific capability mentioned was metal fate and toxicity, though the reviewer making this suggestion

acknowledged that it would be a substantial undertaking. Other more minor enhancements suggested related to data libraries, expansion of GIS capabilities and facilitation of scenario analysis.

Panel Recommendations and OST Responses

Below are summaries of specific comments and suggestions, and our responses to them. The complete written comments are found beginning on page 5 of the Peer Review Report (attached).

Charge Area A: Scientific basis of the enhancements to AQUATOX Release 3 (e.g., consistency with ecological literature, appropriate ecological processes and mathematical formulations, improvement in simulating ecological fate and effects, improvement in applicability to different waterbody types, additional processes, simplifying assumptions, appropriate scale)

Generally the reviewers thought that the enhancements did conform to current ecological literature, with the caveat that it is not possible to be entirely consistent, because absolute consistency does not exist. The enhancements have made the model more complete and increased its realism, though it has consequently been made significantly more complex. They did not feel that additional processes should be added (with the possible future exception of metal fate and toxicity). They offered a few comments about specific processes (see below). They felt that the simplifying assumptions were reasonable and well-documented, though it is the responsibility of the user to determine when particular assumptions are valid for their application. Overall, they felt that the enhancements have significantly improved the scientific basis and utility of the model.

Comment: The first section of the documentation needs to describe the timestep, the conceptual approach (fugacity vs. continuous vs. discrete) and the output resolution (site integration, outlet representation, etc).
Response: Much of this information is in the Technical Documentation already, but it is scattered among several sections. We will expand the introduction to include this information, and include references to the relevant chapter.

Comment: One reviewer suggested a series of more detailed peer reviews for different aspects of the model (ecological, toxicology, fate/effect). He acknowledged that the level of effort would be substantial.
Response: As the reviewer acknowledges, this would require a significant expenditure of resources. Although the suggestion has merit, we feel that for the foreseeable future it would be best to concentrate on expanding the variety of applications of the model, though possibly with additional review of applications as they are done.

Comment: One reviewer thought that Ecological Stoichiometry isn't discussed explicitly in the Technical Documentation.
Response: This information is already in the Technical Documentation, though it may be a bit "buried" in the document, and needs to be reviewed for clarification, and expanded, particularly to include a mechanistic explanation. We will review and edit as necessary.

Comment: Oxygen saturation is slightly lower than those shown for pure water.
Response: We re-evaluated the construct governing oxygen saturation, and it was found to yield lower values than the commonly used APHA (American Public Health Association) construct; we decided that the APHA construct was preferable. The change has been made in the code, and the technical documentation will be updated.

Comment: One reviewer felt that the limitation of pH to 8.25 as an upper value could limit its prediction capabilities, as many natural waters exceed that pH, at least late in the afternoon. This reviewer offered a possible alternative model that may work.
Response: The current construct was chosen, despite the upper limit of 8.25, because of its relatively small data requirements. We also recognized that a pH of 8.25 was a threshold for the carbonate system and that exceedance, although not quantified, was sufficient for modeling most responses including carbonate precipitation and biotic stimulation. We will investigate the suggested model to see if its approach would be a viable alternative for systems with higher pH.

Comment: One reviewer expressed a concern with a possible issue of mass balance of toxicants, particularly when multiple contaminants are present at high concentrations in sediments. There appears to be no upper limit to the binding capacity of sediment, and that the model assumes no "competition" for sorption sites for multiple toxicants present at the same time.
Response: We suggest that this is not, per say, an issue of "mass balance" but rather pertains to "toxicant fate" processes. The AQUATOX model strictly tracks mass balance of toxicants, and this concern really pertains to where the mass is predicted to reside during the simulation.

The binding capacity of sediments is limited to the equilibrium concentration by the limit on sorption as equilibrium is reached (Equation **(352)** in the *Technical Documentation*). Furthermore, the mass of the sediments are considered so that the maximum mass of chemical that could be sorbed to the sediments is equal to the mass of the sediments multiplied by the equilibrium concentration in sediments.

The reviewer suggests that at very high concentrations, the assumptions of equilibrium partitioning may break down as the physical limitation of the sediments is approached. We will consider modeling such a physical saturation in future versions. Currently, the model should be applied in sediments where the assumption of the chemical maintaining an equilibrium concentration within sediments is defensible. (Incidentally, the model has never been applied where partitioning data suggest that the contaminants have exceeded saturation in the sediment, even though it has been applied at a highly contaminated SUPERFUND site). In highly contaminated sites, the derived chemical *KPSed* value should be evaluated against site-specific data. (This value may also be overridden within the AQUATOX GUI if site-specific data suggest that a lower value would be more appropriate.)

Given that the model does not calculate a physical saturation of chemical in sediments for a single chemical, it follows that this limitation also does not apply for multiple chemicals. The reviewer is correct to point out that in future versions, if such a limitation is imposed, it would be best to consider multiple chemicals to produce the most robust formulation.

Comment: One reviewer expressed concern over the use of octanol water partitioning coefficients (Kow's) in partitioning for dissolved organic material (DOM), and the explanation in the accompanying documentation. He provided several references as suggested additions.
Response: We will review the existing documentation for opportunities for clarification, review the references provided, and incorporate them if necessary.

Comment: One reviewer strongly recommended development and inclusion in the technical documentation of a "mission statement" for AQUATOX, which would describe its intended use, strengths and limitations, the need for ground-truthing at the level appropriate for where, when and why it is being applied, as well as the fact that it is being continually updated and refined. A "user-beware" sentence should also be included within the mission statement to explicitly state that the model is not intended to be used in a "plug-and-chug" fashion. Rather, the model and its case studies should be applied on a case-by-case basis in the context of its intended use.
Response: We agree that such a cautionary statement would be highly informative to users. A draft has been completed and will be incorporated into the Technical Documentation.

Comment --- One reviewer suggested that we evaluate an overall "energy budget" for biomass in a system; i.e. whether there is the possibility of exceeding a system's overall carrying capacity, possibly when there is significant immigration and/or emigration.
Response: This is an interesting suggestion, and we may do this type of analysis sometime in the future. However, we believe that there is sufficient feedback in the model so that exceedance would only be short-lived, as in nature.

Charge Area B: Reasonableness of the model's predictions (accurate ecological processes, level of validation, enhancements to uncertainty and sensitivity analysis tools)

In general the model predictions appear reasonable, but specific applications, especially to new types of systems, will need calibration and validation. The extent required will be dependent upon the purpose of the modeling exercise, and its possible implications or consequences. The panel felt that they needed more validation examples, and they recommended providing this info in the documentation or on the web site. Efforts in the near future should focus on additional calibrations and validations. The panel also recommended specific areas that needed expansion or explanation with regards to uncertainty and sensitivity analysis.

Comment: One reviewer suggested evaluating intrinsic model uncertainty, as opposed to parameter and driver sensitivity.

Response: Intrinsic model uncertainty may be defined as uncertainty due to model formulation and numerical description. One manner of evaluating intrinsic model uncertainty is to examine alternative models. For several AQUATOX processes there are alternative constructs that can be chosen by the user. These include whether or not there is adaptation by algae to light, whether internal or external concentrations of toxicants are used to compute toxicity, and whether or not lipid content is computed dynamically. For these alternative constructs the user can compare the results of the two alternative formulations.

However, to expand the model with additional alternative constructs would require significant formulation and programming resources. Furthermore, alternative formulations provide an imperfect measure of intrinsic uncertainty as both models could have common conceptual or mathematical errors. One recent literature article notes "While intrinsic model uncertainty is very well understood, quantitative assessment of this source is hardly possible.[1]"

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[1] Erechtchoukova, M.G. (2005), Uncertainty transformation in ecological simulation models, International Congress on Modelling and Simulation MODSIM 2005 (A. Zerger, and R.M. Argent – eds.), December 2005, Modelling and Simulation Society of Australia and New Zealand, pp. 22477-2483, Melbourne. http://www.mssanz.org.au/modsim05/papers/erechtchoukova.pdf

Comment: The panel recommended that the discussion of calibration and validation be expanded, to include a synopsis of calibration and validation techniques, as well as metrics for goodness of fit for calibration and validation.
Response: We will review the current material and expand the discussion; including a presentation of the weight of evidence approach we have adopted in several applications to evaluate model performance. We are also finalizing a new Technical Note that acts as an example of calibration and verification of AQUATOX; it will soon be released on the AQUATOX web site. However, a textbook discussion of calibration and validation is beyond our scope.

Comment: Additional explanation of the tornado diagrams is needed. In addition, the panel recommended developing guidance on choosing appropriate parameters in order to perform the sensitivity analysis.
Response: We will review the existing text and expand. We are in the process of doing a systematic sensitivity analysis of the model, and once that is completed, it will help us develop guidance on choosing appropriate parameters to test.

Comment: Add discussion of the assumed independence of parameters in the sensitivity analysis, and its implications.
Response: We will review the existing description and add information about the independence of parameters assumption and the fact that the uncertainty analysis routine may be used for sensitivity analysis of correlated parameters.

Charge Area C: Suitability of the model for application to federal and state government decision-making, particularly water management programs and regulatory programs such as TSCA. (e.g. sufficient verification and documentation, flexibility, applicability to multiple waterbody and stressor types)

The enhancements to Release 3 have made AQUATOX even more flexible and suitable for regulatory purposes. It can be applied to such programs as TMDLs, water quality criteria development, ecological risk assessment, and for analyzing pollution control scenarios, though as one of several analytical tools, not alone. Site-specific applications will likely need calibration and/or validation. In particular, additional validation is needed for application to chemical toxicants. As more validations are performed greater confidence can be placed in the model predictions.

Comment: The panel strongly urged development of an upfront statement to explicitly describe what is and what is not known about the model's degree of validation. They suggested development of an overview document, with links to available material, possibly including prior validation reports.
Response: We agree that a summary of what has been done to validate AQUATOX would be a very useful document. Some material on this subject already has already been developed for other purposes (such as the training workshops), which could be expanded to include discussion of purpose and model domain, etc. The AQUATOX web site (http://www.epa.gov/waterscience/models/aquatox/) already has links to download the four existing validation reports done for earlier model versions, as well as a bibliography of journal articles about AQUATOX. In particular, Park et al. (2008) has a section on calibration and validation of the model.

Material specifically addressing and summarizing the extent of validation would be a valuable addition to the web site and/or Technical Documentation.

Comment: One reviewer felt that the model has not been sufficiently validated for chemical toxicants.
Response: Most of the focus within the Office of Water in the past several years has been on nutrients and related stressors, with much less on chemical toxicants. We agree that additional applications to, and validation efforts for, chemical toxicants would be very desirable before the model could be considered well validated. However it should be recognized that validation is an iterative process, and the degree to which a model can be considered "validated" depends to a large extent on the purpose of a particular application. The model has been validated for several chemicals in a variety of aquatic ecosystems, and we will make that clear in the Technical Documentation.

Comment: The model should be used as one tool among several for many regulatory applications. In particular, any site-specific application would need calibration and/or validation against site-specific data. It may be useful to augment the existing technical approaches currently used for applications such as water quality standards and criteria development, and for inferring causal relationships between stressors and aquatic effects.
Response: We agree that the model should not currently be relied upon as the sole determinant of most regulatory applications. One reason is that generally there isn't sufficient monitoring data to gain a high degree of confidence in the results. In those cases where it has been used, such as evaluation of proposed water quality criteria, it has been as one part of the analysis to evaluate potential biological responses and interactions. As the model gains a greater "track record", and where there is sufficient site-specific data, increased reliance on model results should be possible.

Charge Area D: Overall utility of AQUATOX Release 3 (data needs, default data, incorporation of ICE, user friendliness, suggested improvements)

The reviewers appreciated the default data libraries, and the ability to modify them when necessary. They recognized that the data needs are large, and that the temptation would be to use only the data libraries and not get more site-specific data when needed, or to otherwise evaluate whether the defaults are appropriate for a given application. They felt that the user interface was very user friendly, especially for such a complex model, and that the enhancements have improved the overall utility of the model. They thought that the additional tools (enhanced graphical output, sensitivity analysis, ICE, unit conversions, and the context-sensitive help files) were all valuable and useful tools.

Comment: One reviewer stated that the most challenging data needs are biological community structure, and that there was a danger of users incorrectly assuming that the list of species in the libraries were present in their ecoregion. He recommended that we develop libraries for each third-level ecoregion and reach order/water body type within those ecoregions in order to appropriately build the biological communities.
Response: We agree that increasing the geographic coverage of libraries and studies is highly valuable, and where possible we are already doing that. The suggestion to systematically develop

default biological communities for each third-level ecoregion is a good one, although it would require significant resources.

Comment: One reviewer suggested that the documentation discuss the influence of different drivers for applications and driving input parameters of each submodel; this would in turn would permit users to focus on the most important data inputs.
Response: We agree that such a discussion, whether in the model documentation, or as a separate guidance document, would be useful. The ongoing sensitivity analysis should provide input for such a document, as well as existing workshop materials that address the issue.

Comment: All of the reviewers appreciated the inclusion of the toxicity estimation tool ICE (Interspecies Correlation Estimator), though they emphasized that it should not be used blindly. One reviewer specifically suggested that all extrapolations using ICE include the uncertainty or probability from the regression equations factored into any other risk assessment. There could also be a discussion of other sources of toxicity data for AQUATOX.
Response: We are reviewing the statistics used in Web-ICE to ensure that all appropriate statistics are imported into AQUATOX. We will also develop or expand the documentation concerning other toxicity data, possibly as part of the new section on data sources (see below).

Comment: One reviewer mentioned that the unit conversion utility is unique, valuable, and that it would make the development of macro-driven implementation of the model from standardized databases easier.
Response: The diverse extent of AQUATOX parameters required for a specific model implementation likely makes a macro-driven model implementation from standardized databases impractical (e.g., trying to automatically gather data about nutrients, biomasses, ecological state variables, water volumes, and labile content of organic matter would not be straightforward). This suggestion further draws to mind the reviewer's comments cautioning against "plug and chug" model applications. Finally, linking to standardized databases would require significant programming resources and could carry the danger that database structures could change with time. (An example is the linkage to USGS discharge data and conversion to metric units; shortly after the linkage was programmed in AQUATOX USGS changed the file structure to a more flexible format, canceling out most of the benefit of the linkage.)

Comment: One reviewer suggested that we develop "warning flags" for when users enter data that is outside of a given range.
Response: We agree that this would be very useful, though it would require a large effort to develop the ranges for all of the many model inputs. Such checks do exist in the model for a few critical parameters.

Providing additional information to users about parameter ranges and sources will continue to be quite important, however. For example, this type of information can then be propagated into sensitivity analyses and uncertainty analyses. For this purpose, we plan to expand the width of comment fields to allow the conveyance of more information from model developers to model users.

Comment: Develop the capability so that multiple scenarios can be run sequentially (or concurrently on fast machine) rather than just control and perturbed.
Response: The basic capability might not be too difficult to program, but there are many interface implications, and additional tools would be required to manage scenarios, name the scenarios, manage the difference graphs, storing and loading of studies, etc.. We will look into the matter.

However, an easier alternative, at least initially, might be to improve the existing batch mode routine; for example, by allowing the batch mode to export to the same Excel file.

Charge Area E: Features of the supporting documentation (Technical Documentation, Users Manual, context-sensitive Help files)

All of the reviewers thought that the model documentation was well-written, clear and thorough. They offered a few suggestions for additional features.

Comment: One reviewer suggested that we create active links from the context-sensitive help files to the appropriate section of the Technical Documentation.
Response: We agree that more references to specific sections in the Technical Documentation would be valuable to the user and we will add more such references. However, we do not intend to add hyperlinks, as hyperlinks are in general too ephemeral and difficult to maintain.

Comment: One reviewer suggested that the Technical Documentation be made more modularized with the chapters being stand-alone.
Response: We disagree, as the task of modularizing the document would be extremely labor intensive, and probably of relatively low value. We do not anticipate frequent updates to the model or the documentation. For at least the foreseeable future we want to keep the model as stable as possible and focus on model application and validation. We anticipate that we will handle updates as they have been in the past (e.g., Release 2, then 2.1, etc, with appendices to the Technical Documentation). We plan on adding parameter libraries, example studies, etc, as usage expands, but these can be done through the AQUATOX web site and listserver.

Comment: Compare with other models in Introduction of the Technical Documentation
Response: We agree. Much of this information has already been developed for training materials, and it will be easy to incorporate into the document.

Comment: One reviewer requested that we provide the Users Manual as a PDF file as well as the context-sensitive help files.
Response: We agree, and will provide PDF files of both the Users Manual and Technical Documentation.

Comment: Develop a separate section in the Users Manual on data sources. Break it up into parameters, monitoring data sources, etc. Also include a section on data conversions (flow regressions, etc).
Response: We agree that this would be useful. Some guidance on data sources has already been developed for training courses, and the material can easily be incorporated into the Users Manual.

Comment: One reviewer requested more emphasis on the tutorial, perhaps by changing its placement in the Users Manual.
Response: We will develop an expanded tutorial (possibly two), in order to make it more comprehensive. We will consider linking it to the "case study document" as that is developed.

Charge Area F: Additional enhancements

Aside from suggestions made earlier in the review, the primary enhancements suggested were to expand GIS capability and add metal toxicity. In the near future, the reviewers recommended that our efforts emphasize model validation, user support, and documentation.

All future enhancements will require further examination and consideration, and will depend upon available resources, and the value added for the primary users of the model.

Comment: One reviewer suggested additional integration with GIS.
Response: This could be a very substantial effort. We have already submitted a proposal to NASA, which if funded could certainly help with additional linkages to GIS data layers. We may also want to re-evaluate the BASINS 4 linkage for additional opportunities.

Comment: Add metal fate and toxicity.
Response: As acknowledged by the reviewer, this would require a substantial level of effort. However, it has been a recurring suggestion over time, and there is a fairly significant interest in it. It will continue to be on our list of potential future enhancements. There may alternative approaches, rather than attempting to handle metals in a similar fashion to organics, for example linking AQUATOX to a model such as MINTEQ, and then using external toxicity rather than internally-based toxicity. This was done with copper in an application in Evers Reservoir, FL. With regard to mercury, it may be possible to model the bioaccumulation of mercury, if the user can supply sufficient observed methyl Hg concentrations to drive the simulation. In other words, rather than having AQUATOX simulate the methylation processes explicitly, the user would provide the MeHg available for uptake and bioaccumulation. If interest in metals, and in particular, Hg, continues, and if we have sufficient resources, we will investigate this approach further.

Attachment