

ATTACHMENT

PEER REVIEW COMMENTS and EPA RESPONSES

GENERAL COMMENTS FROM PEER REVIEW PANEL

Don DeAngelis

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 not perfect, but it is a major step on the road to improve quantitative assessments of such impacts. I believe that it can be used now in many situations, at least as an information input to decisions concerning particular stressors. Any critical comments that I make below should be taken in the context of my general opinion that *AQUATOX* is ready now for some applications and, with appropriate calibration and testing, could be used in a wide variety of applications regarding regulatory decisions.

Rob Pastorok

AQUATOX is a valuable tool for analyzing environmental issues related to aquatic systems. Although the review below points out areas for improvement, the current version of the model is ready for implementation in a regulatory context as long as sufficient calibration and testing is done for specific applications. The model represents the structure of complex aquatic systems well. *AQUATOX* is probably the most complete model of its type described in the literature. The version reviewed treats aquatic systems as homogeneous along the horizontal dimension, but a segmented model for application to rivers is available. *AQUATOX* contains many features and is very flexible. In most cases, the general predictions of the model appear to accurately reflect ecological processes and behavior in aquatic ecosystems.

Frieda Taub

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. It is particularly useful in exploring the sensitivity of predictions to model parameters with varying degrees of uncertainty. Like all models, it makes simplifying assumptions and therefore is vulnerable to challenge if a regulated party objects to the outcome. For regulatory decisions that are not site specific, the model may be useful in its present form (e.g., for regulatory programs such as TSCA which make decisions based on QSAR predictions). For site specific predictions, a great deal of calibration may be required before the model can be used. In site specific cases, the current complexity of processes may be increased or condensed as appropriate. The model uses regressions from toxicity measurements on a few, well tested species, to estimate the toxicity to a variety of other species; these estimates might not be representative of the toxicity that would be experienced by site-specific biota. It would be wise to compare the model output to data sets of analytical results from field studies designed to study the fate and effects of pesticides; a number of these studies are available in the literature (Fairchild, et al., 1992; Graney, et al., 1994; Heinis and Knuth, 1992; Hill, et al., 1994; Lozano et al., 1992; Webber, et al., 1992).

Response

It should be clarified that the segmented version (called "Release 3" for the purposes of this memo) is essentially complete, but not publically available yet. The segmented version was developed for the SUPERFUND program, for the Housatonic River, MA PCB cleanup project, which is subject to litigation. It has not yet been decided how and when to release the segmented version of AQUATOX publicly.

We agree with and appreciate the remarks concerning AQUATOX's completeness and usefulness. We also agree that site specific, species-specific data and calibration would be necessary, the extent depending upon the purpose of the given application and the consequences of the outcome (more detail appears in the individual comments and responses in the attachment).

RESPONSES TO SPECIFIC CHARGE QUESTIONS and EPA RESPONSES

(Note: in some cases redundant recommendations have been combined or edited for clarity)

Charge Area A: Conceptual design and scientific basis of AQUATOX

A1: The technical documentation provides the overall technical and theoretical basis of the model, its processes and formulations, and model design and concepts.

- ***Is the information provided in the Technical Documentation consistent with ecological literature?***
- ***Are the processes and mathematical formulations, as described in the technical documentation, appropriate and do they accurately reflect ecological processes?***

Summary of Comments

The processes included in the physical and chemical fate modeling are comprehensive and, in some cases, innovative. Each assumption in the technical documentation is sufficiently documented and is reasonably defensible. All the reviewers agree that the technical documentation for AQUATOX, including its processes and assumptions, is consistent with ecological literature. The technical documentation shows that all the assumptions are based on tested scientific model formulations of ecological processes and are backed up by references to scientific publications, with some additional reliance on professional judgment where necessary. The mathematical formulations of the model are appropriate and accurately reflect ecological processes.

Recommendations and EPA Responses

- **Recommendation:** Explore elaboration of AQUATOX as a teaching tool for ecosystem ecology courses.
Response: This is outside the immediate purposes of the Office of Science and Technology and Office of Pollution Prevention and Toxics, although we agree that it could be well suited

for that purpose, and perhaps could be useful for training of risk assessors and managers on fate and effects models.

- **Recommendation:** Clarify representation of detrital food web in technical documentation.
Response: We will include additional explicit discussion of the detrital food web in the technical documentation
- **Recommendation:** The model uses common mechanisms for predicting the effects of most organic chemicals, which may not actually predict the fate of individual chemicals at individual sites. Sensitivity testing of individual parameters may help to clarify the accuracy of site-specific predictions.
Response: We agree that sensitivity analysis on the chemical fate parameters could be very useful to determine whether the default parameters are valid at a given site, or need site specific values or calibration. This could be of particular importance to parameters that are difficult to measure accurately, such as the octanol-water partitioning coefficient or Henry's law constant. The user can now test the sensitivity of virtually all parameters and loadings by means of the uncertainty analysis utility. (We have just expanded the parameter list, and modified the interface to make it easier to navigate.) Chapter 5 of the User's Manual identifies some of the parameters most likely to be very sensitive; we will review this discussion to see if it merits expansion.

A2: Can the model represent the combined fate and effects of multiple stressors in aquatic ecosystems, including eutrophication, aquatic life effects, ecotoxicology, food chain effects, and bioconcentration/ bioaccumulation/biomagnification of organics?

- **Does the model have sufficient and appropriate ecological compartments and state variables?**
- **Does the model have sufficient and appropriate ecological processes?**
- **Should other state variables or processes be added?**
- **Are some state variables or processes unnecessary for purposes of the model, and should they be deleted?**

Summary of Comments

One reviewer commenting on this question noted that the mechanisms to represent the effects of multiple stressors in aquatic ecosystems largely exist in the model; however, *AQUATOX* might not represent some effects, such as eutrophication, sufficiently, because it does not maintain a strict mass balance of nutrients. Another reviewer felt that it was not possible to determine whether the model accurately predicted the effects of multiple stressors in aquatic ecosystems because there are few published studies on this subject.

The reviewers agree that *AQUATOX* appears to be comprehensive and sufficiently represents the structure of complex aquatic ecosystems that are homogeneous along the horizontal dimension. This is true especially for the 1-D or vertically stratified cases. The model uses regression analysis to estimate toxicity data for species where no such data is available.

The ecological processes modeled in *AQUATOX* are sufficiently complex to account for important biotic and abiotic interactions, but site-specific uses of the model might require that additional processes be considered. The ability of *AQUATOX* to model processes for biological guilds in several trophic levels and associated feedbacks is excellent

With regard to potential additional state variables and processes, one reviewer commented on the many features of *AQUATOX* and its flexibility. The reviewer suggested adding the effects of wave agitation on macrophytes. Another reviewer noted that adding more detrital components might be useful, pointing out that the developers of *AQUATOX* are already in the process of adding these components.

The two reviewers commenting on the question of removal of variables agree that some variables might be unnecessary and could be removed, but only on a site-specific basis. The variables should be retained in the *AQUATOX* model as a whole, thereby keeping its current detail and flexibility.

Response

The comment about eutrophication deserves a response. It is true that not every process related to nutrient cycling and eutrophication is represented completely, and strict mass balance may not be maintained. For example, although macrophytes may release nutrients into the water column, the nutrient uptake from sediments by macrophytes is not modeled explicitly. However, this is meaningful only at those sites where the excluded processes are significant to the functioning of the system; if they are not a significant process, the loss of exact mass balance would not be important. In addition, as one reviewer pointed out, even in those sites where the excluded processes are important, *AQUATOX* could still be used to compare relative changes in various nutrient loading regimes.

Recommendations and EPA Responses

- **Recommendation:** *AQUATOX* should be used as a tool for revealing ecosystem changes that may happen, not making accurate predictions about specific changes in variables, especially indirect effects.

Response: 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.

- **Recommendation:** *AQUATOX* should document and provide cautionary statements about what processes and fluxes are ignored or approximated.

Response: Agree. The technical documentation generally identifies simplifying assumptions and ecological processes that are excluded from the model. However we will review the documentation for opportunities to make it more explicit.

- Recommendation: One possible enhancement would be the ability to model more than two sediment feeders.

Response: This is unnecessary, as the user can already model multiple sediment feeders by correct parameterization of benthic organisms to make more than two groups “eat” sediment detritus; in essence by “fooling” the model. We can add text to the user’s manual about this and other “modeler’s tricks and tips”.

- Recommendation: Future enhancements to allow segmentation will improve the ability of *AQUATOX* to model rivers and spatially heterogeneous lakes and reservoirs.

Response: The segmented version (called Release 3 for the purposes of this memo) will allow multiple, linked simulations extending down multiple reaches of a river. In addition, *AQUATOX* Release 2 allows for a certain amount of horizontal heterogeneity by means of percent littoral area, area available for macrophyte colonization, and the new habitat disaggregation constructs that allow the assignment of animal species to a given type of habitat (run, riffle, or pool). Any attempt to add more spatial segmentation would have to be balanced against the increased requirements for input data and most likely would require linkage to a hydrodynamic model.

- Recommendation: When *AQUATOX* is used to address site-specific issues, the inclusion of additional ecological processes might be necessary to provide accurate results.

Response: We agree. Knowledge of the site, and assurances that important processes are included, should be part of any modeling exercise. The decision as to what processes to include depends not only on the site but on the purposes of the analysis. It should be noted that addition of more ecological processes may lead to additional input requirements, as well as potential sources of uncertainty, so the need for additional processes for realism must be balanced against the cost. As the developers work with site-specific applications they have routinely been adding processes as needed.

- Recommendation: Simplify the model for specific applications.

Response: The user can already simplify a study file to a very simple, even abiotic, system by deleting all biotic compartments. . If this recommendation is for customization for particular applications or for particular programs (e.g. a screening tool), this could probably be done, once the specific objectives are defined.

- Recommendation: Add effects of wave agitation on macrophytes.

Response: We agree that this could be a useful addition for those sites where wave agitation has a significant impact on macrophytes; however as the reviewer pointed out, this is not likely to be the case at very many sites. It could be added to *AQUATOX* with relatively small effort; and would not likely add to data input requirements. Therefore we shall add it to the list of future enhancements that can be added as the need arises.

- Recommendation: Add more detrital components.
Response: AQUATOX Release 2 already has eight detrital compartments, which is more than most models. The eight are: refractory and labile sedimented, dissolved, particulate and buried. Release 3 (segmented version) has additional compartments, but consequently the data input requirements are higher for Release 3. Indeed, many current users express discomfort with the current number of compartments; to add more might be counter-productive with regard to increasing usage of the model.

A3: Are the simplifying assumptions reasonable?

Summary of Comments

There is unanimity among the reviewers that the simplifying assumptions are reasonable. One reviewer noted that the empirical relationships used to reduce the complexity of the model were a good addition to the model. Another reviewer pointed out that the assumptions are reasonable but might not fit specific examples, and the user would need to determine which of the parameters are not realistic. One of the assumptions that might pose a problem is when the model assumes that if all invertebrates are killed, the fish in the system will starve and the food chain will collapse.

Recommendations and EPA Responses

The comment on invertebrates and the food chain deserves a response. An inappropriately “collapsing” food chain probably indicates that model needs better calibration to that system, with more accurate characterization of food preferences, and of sensitivities of the various prey species to a given stressor. It should be pointed out that what a species actually eats at a given time may not be the same as their preferences; if their preferred food is unavailable they will switch to a less preferred item. Most fish are parameterized to feed on detritus and sometimes plants as well.

- Recommendation: For a teaching model include the complex dynamics of decomposition, in which rates might depend on C:N:P ratios and nutrients are immobilized by microorganisms.
Response: As mentioned in Section A1, enhancement of AQUATOX as a teaching model is outside scope of our work and budget, although the project is certainly feasible. Variable stoichiometry would be a significant increase in complexity.
- Recommendation: Include more detailed treatments of decomposition in later versions of *AQUATOX*.
Response: If there are significant numbers of waterbodies where a more complete characterization of decomposition is required in order for a management decision to be made, we might consider doing this, but we feel that most regulatory applications would not require it.

A4: Does the model operate at the appropriate spatial and temporal scales, and temporal resolution?

Summary of Comments

The reviewers noted that some improvement could be made in the spatial and temporal scales and the temporal resolution; however, the current scales and resolutions are adequate for some cases, such as for natural aquatic communities.

The reviewers offered recommendations on how the model could be improved spatially. They noted that vertical disaggregation of streams into zones of free-flowing water and bottom boundary layers, adding the ability to model more than two sediment feeders, and adding horizontal heterogeneity would be beneficial in estimating the concentrations of nutrients and toxicants in aquatic ecosystems. Allowing segmentation will improve the ability of *AQUATOX* to model rivers and spatially heterogeneous lakes and reservoirs.

One reviewer believes that a temporal resolution of a day is fine, except in cases where there are diurnal variations in oxygen concentration and other values that might effect model performance. Other instances where the temporal resolution might not be appropriate would be modeling tidal changes in estuaries or storm hydrographs in streams and reservoirs. The reviewer suggested that future releases of *AQUATOX* should include options for hourly time steps.

Recommendations and EPA Responses

- **Recommendation:** Migrate towards an option to perform simulation on hourly time steps..
Response: The decision whether or not to add an option for an hourly time step depends on the endpoints of interest, and whether they are sensitive to daily variations. For example, hourly time step could be valuable where diurnal extremes of dissolved oxygen are important, rather than daily averages. In order to accurately simulate these finer processes, however, several other processes would need to be added as a consequence, such as photosynthesis based on hourly light, diurnal migration of zooplankton, and diurnal drift. These would increase data input requirements for the user. As the reviewers point out elsewhere, the need for more processes to add realism must be balanced with the desire for simplicity and to minimize the burden on the user.

The reviewer mentioned tidal cycles as a reason to add an hourly time step option. It may possible May be able to treat tidal variations in a different manner to eliminate the need for an hourly time step, as has been done for the estuarine version, which uses the daily tidal range and freshwater discharge to compute the thicknesses of the upper and lower layers, turbulent diffusion and entrainment of salt water.

- **Recommendation:** Include analogous vertical disaggregation of streams into zones of free-flowing water and bottom boundary layers.
Response: We will add this to a list of potential enhancements to explore. There may be a relatively simple method of doing this, such as a simple function based on channel roughness, as opposed to going to a complicated 3-D representation.

Charge Area B: Reasonableness of AQUATOX predictions

B1: Do the predictions appear to accurately reflect ecological processes and behavior?

Summary of Comments

As noted previously, the reviewers found many of the individual ecological processes are accurately represented in the model. However, the accuracy of the model for predicting changes to an ecosystem as a whole should be evaluated. All reviewers generally agree that the model predictions seem reasonable and reflect ecological processes and behavior. One reviewer suggested that EPA should define program- and use-specific validation criteria that are based on the level of accuracy required for a particular application. By defining the validation criteria, EPA could set the accuracy expectations for the model output. Additionally, the accuracy of predictions from specific model applications could be predefined and validation processes established prior to running the application. The reviewers noted specific examples of questionable results (i.e., fish and algal biomass predictions and PCB bioaccumulation), which were not clearly resolved in the supporting materials.

Recommendations and EPA Responses

- **Recommendation:** If EPA values the model's ability to provide accurate predictions for all trophic levels in a system, then the discrepancies that currently exist in the model should be resolved (e.g., when appropriate, the accuracy of algal biomass estimates should track with the estimates of biomass for algal grazing fish).
Response: The answer to some of the discrepancies that the reviewer refers to may lie in getting a better calibration for sculpins and alewives (two of the fish species in the Lake Ontario validation), which had not been modeled in AQUATOX prior to this attempt. Also, having better field data against which to compare some of the model predictions would improve confidence in the model.
- **Recommendation:** Include a systematic explanation of each sharp upward and downward jump of fish biomass in the Model Validation Reports.
Response: We do not intend to re-do the validation reports (which were performed with Release 1 of AQUATOX, not Release 2), but in future validations we will attempt to pay more attention to similar patterns and explain them further. Some of the seemingly unrealistic graphs may simply be the result of the time scale on the graphs, or the fact that the lake was undergoing stratification and de-stratification, thus complicating interpretation of the graph.

The developer has revisited the Onondaga Lake application and has gotten a better simulation. As with the other validation reports, the number of state variables that could be validated against observed data was limited by the available data. In addition, a units error in the parameterization of fish respiration based on the Wisconsin Bioenergetics Model accounts for much of the rapid buildup of fish biomass and has been corrected. Routine plotting of rates helps explain and verify model results.

- **Recommendation:** Provide additional explanation in the supporting documents for algal biomass and PCB bioaccumulation predictions.

Response: We could not find this recommendation in this section of the report, however we will review the section of Technical Documentation dealing with bioconcentration and bioaccumulation for opportunities to clarify or expand the explanation.

- Recommendation: Define validation criteria for the model to be used in various applications and establish accuracy levels for the model under different scenarios.

Response: The development of any type of validation criteria is, as the reviewer points out, more appropriate for an individual program than for OST or OPPT as the developing offices. As the reviewers acknowledged, the required precision and accuracy differs both programmatically, and even within a program, as the particular consequences of a “wrong” answer may vary greatly. For example, all TMDLs, or even all nutrient TMDLs, do not need the same level of precision.

It should be noted that as an agency EPA is working on guidance on model acceptability and good modeling practices, including validation criteria as part of the activities of the Council on Regulatory Environmental Modeling (CREM).

B2: Has the model been sufficiently validated and verified to apply it to a variety of water body types (streams, rivers, lakes, ponds, mesocosms)?

Summary of Comments

The reviewers indicated that they believe the model has been adequately verified for a variety of water body types for estimation of water quality and lower trophic level responses. They also noted that the model has been sufficiently validated for flow, nutrients, light, and grazing, as well as dissolved oxygen, algae, periphyton. However, the reviewers all expressed their belief that more validation could be performed for certain parameters, especially biotic elements, and actual biotic-effects data for toxicants.

Recommendations and EPA Responses

- Recommendation: Incorporate additional systems with enough data for calibration and validation, including biotic elements of the model. Use *AQUATOX* to predict the outcomes and compare these outcomes to some specific examples of aquatic communities. Find additional data sets to perform validations against. Validation of the model, especially for toxicant effects on biota, including trophic interactions, needs to be published in peer-reviewed literature.

Response: We agree that more validation is always better, in order to build confidence in and experience with the model. We will consider additional validation of biotic responses to be high priority for future validation work. We also agree that publishing the results in the open literature would be a valuable exercise.

- Recommendation: Use *AQUATOX* to model field studies with information from mesocosm results submitted for pesticide registration, companies that may be willing to release data for model comparison, and EPA-commercial advisory groups.

Response: The Office of Pesticides may be a useful source of additional datasets to test against, when resources are available for additional validation. It is not clear how much historic mesocosm data would be available, however, as mesocosm data are not required for pesticide registration decisions currently.

- Recommendation: Look into the possibility of using confidence intervals in the validation process. Define the associated levels of uncertainty for using the model under various scenarios.

Response: See answer under B1.

- Recommendation: Emphasize the versatility of the model for organizing data related to stressor effects, as well as for making ecological predictions.

Response: We agree, and are about to start a collaboration with NCEA (National Center for Environmental Assessment) within ORD on demonstrating how AQUATOX could be used within the existing stressor identification framework.

B3: Does the uncertainty analysis capability provide a sufficient analytical tool to quantify model uncertainty, environmental variability, and parameter sensitivity?

Summary of Comments

The reviewers like the uncertainty analysis capabilities of *AQUATOX*, but desired more documentation of this feature and its assumptions. Presently, there are no special tools in *AQUATOX* that can be used to perform sensitivity analyses, which can be done manually. The Monte Carlo tool portion of *AQUATOX*, which does not currently address treatment of correlations among variables in the model, needs improvement.

Recommendations and EPA Responses

- Recommendation: Provide a more detailed description of the uncertainty analysis in the technical documentation.

Response: We will expand the description and background information in the revised technical documentation, and expand the instructions in the user's manual on its use (e.g. how best to use it for sensitivity analysis).

- Recommendation: Improve the Monte Carlo simulation features of the model, tools to evaluate correlations among variables.

Response: We are investigating the incorporation of correlations among variables into the uncertainty analysis utility. If it is a relatively straightforward and inexpensive task, we will consider adding this option. It is not clear at this time how often this capability would add significantly to an analysis, but it would be a valuable option for those cases where there are significant correlations between variables at a site. However it must be recognized that it is unlikely that most users would have the information available to quantify the correlation among variables.

- **Recommendation:** Put more effort into comparing toxicant predictions with data and critically examine the variability of data sets.
Response: This comment appears to be related to a potential application of the model, that is, as a possible means to explain the variability observed in sampled data. We agree that this could be a valuable application of AQUATOX, and would enable users to maximize the value of their data.

Charge Area C: Overall utility of the model

CI: AQUATOX has a large number of parameters and requires extensive data input for biological and chemical characteristics as well as site data and environmental loadings. We have attempted to address this by supplying extensive data libraries, as well as developing the extension to the BASINS program.

- ***Comment on the data needs of the model, specifically defaults vs. site-specific data and the user's ability or necessity to obtain or modify the data needs.***
- ***Do the default values appear to be scientifically acceptable?***

Summary of Comments

Reviewers noted that the data requirements of *AQUATOX* are high, and that the default values are helpful in certain circumstances, but should be used with caution. For site-specific models, the default values might lead to errors because site-specific data such as growth rates may differ significantly from the default values. The default values could be used in the initial analysis to see what additional data are needed.

Trophic interactions are a strength of *AQUATOX*, but estimating the toxicity of chemicals to most of the species from only a few species could be risky. Although well documented in the supporting materials, the use of a few organisms for toxicity data and the use of regression analysis to estimate toxicity data for other organisms was cited as a possible weakness of the model.

To use the model in a regulatory context, users would need to evaluate and input many different data points to accurately parameterize and sufficiently calibrate the model.

The default values appear to be scientifically acceptable for their purpose.

Recommendations and EPA Responses

- **Recommendation:** Extend the data set of default parameters.
Response: We agree. We continue to expand the default libraries to include more species, more chemicals, and more site types as we undertake additional applications. We note that, with regard to the comment on variability of biological parameters between sites, the model attempts to use parameters that are relatively global in nature, and not dependent on the site. To use the example from the report, growth rates as predicted by *AQUATOX* are a function of the maximum growth rate, modified by a number of factors such as temperature, food availability, etc. The *maximum* growth rate

of a fish species should be relatively intrinsic to the species, and will be much less variable among sites than the *actual* growth rate.

- **Recommendation:** Add measures of variability (e.g., range and standard deviation) to the data libraries.
Response: This is a good idea, although it would not be a trivial task, and outside of the existing resources. In the interim, there are already fields for measures of variability (minimum, maximum, standard deviation) found on the distribution screens within the uncertainty analysis utility. Currently they are derived from the mean value by default, but may be overridden by the user. We will add notes to the Technical Documentation and the parameter screen pointing the user to the uncertainty screens. We will also add an explanation of the default derivation to the uncertainty analysis section. In addition, we will make additional effort to use the “notes” fields in the parameter screens to document the variability, where available, and encourage the user to do the same when adding data or editing existing data screens. In the future we will consider adding these fields to the parameter screens themselves.
- **Recommendation:** Add references for each data value.
Response: We will do this to greatest degree possible. We are also working on full citations and bibliography for data libraries.
- **Recommendation:** Expand the number of species used for toxicity estimates to reduce uncertainty associated with regression estimates.
Response: We agree that we should expand the number of species in the data libraries to the greatest extent possible. We will consider expending some resources on searching for more available data; dependent upon resources. However it should be noted that the purpose of the regression option is to allow estimates to be made in the absence of species-specific data; users can easily edit existing data or add data for other species if they have it. We will add more text to the Users Manual on working with the data libraries. There is ongoing work within the Agency at the Gulf Ecology lab to improve the regression equations; if possible and appropriate, we will take advantage of that work to improve the estimations within AQUATOX.

C2: Is the interface “user-friendly” enough?

Summary of Comments

The reviewers agree that the user interface is user-friendly and that the *AQUATOX* wizard is helpful. One reviewer feels the model could be improved with an expanded help section, an up-to-date user’s manual and more tutorials.

Recommendations and EPA Responses

- **Recommendation:** Update the user’s manual for the current version; match the discussion in the user’s manual with the version of the model being used.

Response: We agree. We are updating the user's manual and its graphics to match Release 2.

- Recommendation: Expand the user's manual with more tutorials.
Response: We plan to add more example applications on the AQUATOX web site as they become available; we hope to convert at least one into tutorial format. The current tutorial in the User's Manual will be expanded for Release 2.
- Recommendation: The reviewers made several specific recommendations for improving the User's Manual including:
 - a) The user's manual should inform the user that toxicant concentrations are conveniently listed in the output list.
 - b) Warn users of possible scaling issues in outputs that may obscure changes to parameters of interest.Response: We could add more suggestions and "tips" for users, perhaps by means of text boxes
- Recommendation: Provide a trouble-shooting section in the user's manual.
Response: we could add more suggestions and "tips" for users. We may also add a section of "Frequently Asked Questions" to the web site to deal with commonly encountered problems.
- Recommendation: Continued use of the model in courses or workshops (e.g. SETAC) would encourage its use, increase familiarity, and beta-test the model.
Response: Budget limitations have precluded EPA from presenting workshops to date. There are, however, at least two workshops planned: Dr. Park has committed to presenting workshops at the Ecological Society of America in August 2003 and at the Water Environment Federation TMDL conference in November 2003. We will also investigate other means of user outreach and training in the event that budget restraints continue.

C3: The ability to run Control vs. Perturbed, and to determine percent differences, is presented as a means of minimizing the need for extensive site calibration. Comment on this assertion.

Summary of Comments

The reviewers agree that the ability to run Control vs. Perturbed comparisons and to graphically evaluate percentage differences is useful, particularly for comparative or screening analyses. However, in cases of site-specific assessments (e.g., baseline ecological risk assessment at a Superfund or RCRA site), it may also be necessary to do extensive parameterization and calibration of the model for both the site and a reference site. The degree of such parameterization and calibration will depend on the specific objectives of the assessment.

Recommendations and EPA Responses

- Recommendation: Calibration of the bioaccumulation and bioconcentration functions are necessary for site-specific applications of the model.
Response: We agree that many applications will require extensive calibration, including complex situations such as bioconcentration and bioaccumulation.
- Recommendation: Guide users in applying appropriate site calibration based on the intended use of the results.
Response: We could not find this recommendation in the peer reviewers' comments. However, we are working on calibration guidance as a separate document, probably to be released over the web site.

C4: The modular design of the model enables addition or deletion of state variables. Is this appropriate?

Summary of Comments

There is unanimity among the reviewers that the addition and deletion of state variables is useful and increases the flexibility of the model.

Recommendations and EPA Responses

- Recommendation: Have the program summarize the setup so that another user would know immediately if a state variables has been eliminated.
Response: The Wizard already allows display of a summary of all state variables included in the study. The user can also view a listing of all initial conditions. However the reviewer correctly pointed out that by setting a variable to zero, and applying zero loadings, the variable would be effectively eliminated, even though it would still appear in the Wizard summary.

C5: Comment on the utility of the various tools included in the model package

Summary of Comments

- **Uncertainty analysis** - The reviewers think this is an important and useful feature of *AQUATOX*. One reviewer likes the selection of the Monte Carlo analysis and the Latin Hypercube sampling in the uncertainty analysis.
- **Rate saving and output** - The reviewers like the utility; however, one thinks it should be possible to view the rates without having to export them to Excel. Another reviewer likes the flexibility of *AQUATOX* producing output in tabular and graphic formats.
- **Graphing of results** -All reviewers like this function. One thinks there should be a log scale feature and another would like a note added about the date formats on the graph.
- **Wizard** - All reviewers liked this feature.

- **Control setup** - This feature is liked by the reviewers and considered easy to use. This feature makes parameterization of the control simulation easy.
- **Batch mode (quick running of numerous scenarios)** - None of the reviewers used this feature, but they think it would be helpful. One reviewer tried to run this feature but was unable to use it successfully.
- **Ability to run one simulation while simultaneously reviewing the results of others** - The reviewers think this is a useful idea; however, one reviewer wanted clarification whether the modified files were overwriting the original files.
- **On-line help (user's manual)** - The reviewers agree that this is an excellent idea. One reviewer thinks the on-line help should be expanded and another reviewer made several suggestions for on-line support, such as having a Frequently Asked Questions section and updates to data libraries.

Recommendations and EPA Responses

- Recommendation: Indicate that the convention for dates in the graph's time-axis is: month/day/year, not day/month/year.
Response: Actually, AQUATOX does not use month/day/year. AQUATOX uses the short date format as indicated in the users regional settings in windows (CONTROL PANEL, REGIONAL SETTINGS). We will add a note to this effects to the User's Manual.
- Recommendation: Provide users with the ability to directly review rates (i.e., not having to export to Excel).
Response: This could be a useful addition, although it appears that it could result in slower simulation times and decreased performance due to computer resource allocation, particularly on computers without Windows 2000, or on less powerful machines. We will keep it on the list of potential enhancements for a later date.
- Recommendation: Consider the option of using a log scale for the graphical output.
Response: Good idea. This appears to be a fairly simple programming task, and is on the list of enhancements to add in the near future.
- Recommendation: Provide more detailed explanation of batch mode operation and set-up.
Response: We agree; we will add a more detailed explanation to the User's Manual.
- Recommendation: When running one simulation while simultaneously reviewing the results of others, one reviewer wanted clarification whether the modified files were overwriting the original files.
Response: AQUATOX will always detect situations where there is danger that a file will be overwritten and will give the user the option of saving it as another file.

- Recommendation: Expand online user's manual.
Response: We will continue to explore how to improve assistance to the model user, including expansion of the online help features. One possible enhancement is to provide more information on scientific questions (much like having access to the Technical Documentation from the model interface), as opposed to the mechanics of how to operate the model or navigate the interface.
- Recommendation: The Monte Carlo portion of the software needs to be enhanced to be able to deal with correlations among variables in the Monte Carlo analysis.
Response: See answer question B3.

C6: The BASINS linkage is designed to assist in data acquisition, input, and analysis of results. Extensive testing of the BASINS extension is outside the scope of the charge; however, please comment on the purpose and concept, and overall design. Of particular interest is the concept of linking nonpoint source model loadings to AQUATOX.

Summary of Commentss

The BASINS linkage was found to be a good addition because there may be cases where data are already stored in GIS and the data can then be used in *AQUATOX*.

Recommendations and EPA Responses

None.

C7: Comment on potential improvements to any of these tools. Do you have any suggestions for additional tools?

Summary of Comments

The reviewers made several recommendations for enhancements to existing tools and for new tools, as indicated below. However they added the caveat that care must be taken to keep this complex model from becoming too unwieldy.

Recommendations and EPA Responses

- Recommendation: Add a simple tool for graphical representation of food webs.
Response: The same information is currently available in matrix format; this matrix can be printed out if desired. However we agree that a food web diagram could be a useful visual tool. We will investigate how this could be done and the resources required. The suggestion for restricting the lines drawn to those corresponding to preferences over a user-specified amount is a good one.
- Recommendation: Create a model tool that would automatically perform a range of sensitivity analyses, in which each biotic element is varied to evaluate effects on community structure.

Response: This is an interesting suggestion and potential application of AQUATOX, which could increase its usefulness for ecosystem analysis. It is out of the realm of current resources, but we will consider it for future enhancements. In the meantime, in the discussion on how the user can use the uncertainty analysis capabilities (see answer to question B3) it would be possible to add discussion on how to tailor a series of sensitivity analyses to explore different aspects of ecosystem functioning as simulated by the model.

- Recommendation: Develop a tool that quantifies several aspects of biological community stability.
Response: This is an interesting suggestion and potential application of AQUATOX, which could increase its usefulness for ecosystem analysis. It is out of the realm of current resources, but we will consider it for future enhancements. This would entail coordination with the EPA biocriteria program to consider how to best translate AQUATOX output into community metrics.
- Recommendation: Include links to different web sites that provide chemical descriptions.
- Response: Adding links to specific urls from the model itself can be problematic, in part because URLs are subject to frequent changes. However something similar might be done within the AQUATOX web site, as a means of pointing users to sources of data, not only chemical data but flow data, etc. This is beyond the limit of current resources, but will consider it for future work.

Charge Area D: Does AQUATOX provide a sound, credible tool for regulatory decisions, particularly water management programs and regulatory programs such as TSCA?

Summary of Comments

AQUATOX would be a credible tool for regulatory decisions if the results were used appropriately and is one of several sources of information used to make the decision. Proper interpretation of the output from AQUATOX serves as a powerful quantitative tool for making regulatory decisions.

Recommendations and EPA Responses

None.

D1: Has it been sufficiently verified, validated, and documented to apply it to a variety of water body types (streams, rivers, lakes, ponds, mesocosms)?

Summary of Comments

The reviewers agree that more validation together with calibration should be completed. They cited several areas where they feel validation could be improved, such as for mesocosm and fish

biomass parameters. One reviewer noted that in some areas (e.g., fish biomass) more verification could be done. One reviewer referred to the comments made in B2.

Recommendations and EPA Responses

- **Recommendation:** Include additional systems from the literature to calibrate and validate *AQUATOX* against them. More validation should be provided, especially for mesocosms and fish biomass.
Response: We agree that more validation is always better. The amount of validation attempted obviously depends in part on resources, which are quite limited. However we will consider additional efforts for validation of biotic responses, especially in response to toxics, to be high priority for future validation work. The developer is currently working with a dataset that may yield additional validation for fish endpoints.
- **Recommendation:** The relationship of external concentration, internal concentration, and physiological effects should be validated for additional chemicals.
Response: We agree that this would be a valuable subject for additional validation, although it is not clear whether the necessary data are available.

D2: Is it sufficiently flexible to model or accommodate a variety of applications (variety of water body types, stressor types, ranging from general to site-specific)?

Summary of Comments

The reviewers agree that *AQUATOX* is very flexible. This flexibility should support modeling of a variety of water body types and stressor types, as well as various applications from general to site-specific. The inability to model the effects of metals is a gap in the utility weakness of the model.

Recommendations and EPA Responses

- **Recommendation:** Improve the utility and flexibility of *AQUATOX* by adding the ability to model for modeling the effects of metals.
Response: We agree that modeling metals would be a powerful addition to *AQUATOX*'s capabilities, given the number of waterbodies impaired by metals. However it would be a sizeable undertaking, and at the current time it is beyond the available resources.

D3: Is it flexible enough to assess chemicals with a minimum amount of data as well as those that have a robust data base?

Summary of Comments

The reviewers believe that the model is flexible enough to handle sparse data sets and capable of modeling chemical fate for compounds with robust data sets. Two reviewers, however, questioned the use of a complex model for regulatory purposes when data are sparse because the model output might be subject to criticism.

Recommendations and EPA Responses

- **Recommendation:** Emphasize the need to qualify assessments when minimal data sets are used.
Response: We agree that training and guidance materials should stress appropriate application and limitations of models

D4: Can it be used for

- ***establishing a causal relationship between chemical and physical stressors and their combined, direct, and indirect effects on aquatic biota?***
- ***ecological risk assessments of organic chemical stressors, nutrients, etc?***
- ***development or assessment of water quality criteria (BAFs, numeric WQC for nutrients)?***
- ***TMDL analysis and development, specifically the derivation of water quality targets, and required load reductions?***
- ***identification of which stressor among several potential stressors is causing impairment of aquatic life?***
- ***analysis of alternative pollution control scenarios and restoration strategies, both short- and long-term?***

Summary of Comments

AQUATOX can be used to show possible causal relationships and to evaluate the sensitivity of response variables to various stressors. However, it cannot be used to prove such relationships. The results of a model simulation using *AQUATOX* might contribute to the weight of evidence that certain causal relationships exist.

All the reviewers agreed that the model can be used for ecological risk assessments. The model is useful for assessments on a broad scale (e.g., national evaluations), as well as for site-specific decisions as long as sufficient parameterization, calibration, and testing are done for the site-specific cases.

It may be possible to use *AQUATOX* in developing or assessing water quality criteria, but the model processes may not be applicable to all scenarios. The model might be more useful in determining the outcome of the impacts from setting criteria at specific levels.

The Reviewers presented differing opinions on the use of *AQUATOX* to develop TMDLs. One noted the model would be useful as a means of displaying the contribution of various sources and showing the uncertainty analysis of various scenarios. However, another reviewer thinks it might be difficult to use the model for TMDL development because *AQUATOX* does not maintain a strict mass balance of nutrients, which makes it difficult to use the model to define a TMDL precisely. *AQUATOX* could be used, however, to evaluate the implications of setting TMDLs within a specific range and to evaluate the effects of load reductions. Overall, *AQUATOX* could serve as one part of the decision-making process for developing TMDLs.

The reviewers agree that *AQUATOX* can be used to help identify which stressor among several potential stressors is causing impairment of aquatic life, with caution. The model could support empirical assessments of which stressor is causing the impairment, but it might not work on every system.

The reviewers agree that *AQUATOX* could be used for analysis of alternative pollution control scenarios and restoration strategies, both short- and long-term. The model could be used to evaluate the effects of load reductions singly or in combination, including variation in the magnitude of the reduction. One potential use for evaluation of restoration strategies is to manipulate the recruitment variable to be able to simulate stocking or transplanting. *AQUATOX* could also be used to evaluate changes in substrate types or other manipulations of physical habitat as part of a restoration strategy.

Recommendations and EPA Responses

- **Recommendation:** Add an “optimal control” feature that allows TMDLs to be calculated based on a prescribed set of criteria.
Response: This could be a useful feature to explore in the future, to assist TMDL modelers; a similar feature could also be valuable for applications in which specific environmental goals are being sought; e.g. a specific numeric water quality concentration of a pollutant.
- **Recommendation:** Include documentation and cautionary statements for the processes and fluxes that are approximated or not included in the nutrient mass balance.
Response: We agree that, although the information for the most part is already there, the documentation could be more explicit about which processes are or are not included. This would allow a user to more easily determine the suitability of *AQUATOX* for a given situation. This could be particularly meaningful at those sites where the excluded processes are significant to the functioning of the system; if they are not a significant process, the loss of exact mass balance would not be important to the analysis.

Charge Area E: Documentation: Organization, clarity of presentation, utility as a reference, and accuracy.

E1: Comment on the user's manual, including the addenda (draft) and the on-line help version of the user's manual.

Summary of Comments

The user's manual is well written, but there is need for additional clarification. The model output units should be explained better to the reader in the user's manual.

Recommendations and EPA Responses

- Recommendation: Clarify some parts of the documentation and technical manual, especially on the uncertainty analysis and the ecotoxicology portions of the model. The section of the user's manual on uncertainty analysis could be expanded to include examples of using *AQUATOX* in a risk analysis context.

Response: Expansion of the uncertainty analysis and ecotoxicology portions of the documentation is already in progress.
- Recommendation: A section of the user's manual dealing with modeling approaches should be added, including references to more detailed discussions of modeling strategies written by others. Users of *AQUATOX* have the capability of modeling a specific ecosystem in different ways, depending on the available data and desired outcomes. Guidance in the user's manual to help modelers to decide on modeling strategies would be helpful.

Response: We agree that additional guidance on modeling technique could be very useful. We may do this in a variety of ways, such as through a text boxes for minor "user tips", a separate section in the Users Manual, and by separate technical notes that could be released as separate documents. We currently have a technical note on model calibration techniques in draft. We will also put examples of how *AQUATOX* has been applied in different situations onto the web site as they become available. However, it is not the intent of the *AQUATOX* user's manual to provide extensive guidance on modeling in general.
- Recommendation: The flexible aspect of *AQUATOX* allowing a user to reassign compartments to different guilds and parameterize compartments as desired could be explained in detail in the user's manual, including examples of realistic food web structures.

Response: We agree; we can add this as one of the "user tips"
- Recommendation: Provide a separate document on objectives of regulatory programs in which *AQUATOX* would be used and ideas on use of the model in the context of various regulatory programs.

Response: We agree that it is a good idea to present ideas and examples of how *AQUATOX* can be used in various regulatory programs. Rather than preparing a separate document, however, we plan to add more example applications and case studies in a variety of regulatory program situations to the web site as they become available.

E2: Does the technical documentation, including addenda

- provide the overall technical and theoretical basis of the model?***
- provide processes and formulations?***
- provide sufficient model design and concepts?***

Summary of Comments

The technical documentation is well organized, there are several small errors and sections of the technical documentation that are not clear.

The reviewers agree that the technical documentation provides the overall technical and theoretical basis of the model. However, in many places the text could elaborate on certain concepts, such as, using equilibril bioaccumulation factors (BAFs) or bioconcentration factors (BCFs) to constrain model calculations, even though the model is actually dynamic (nonequilibril).The rationale for the use of internal concentrations in the ecotoxicology component could be explained further.

The reviewers agree that the technical documentation provides processes and formulations. The reviewers feel that the technical documentation provides sufficient model design and concepts. One reviewer, however, noted that a section on uncertainty analysis should be added.

Recommendations and EPA Responses

- Recommendation: Upgrade technical documentation by incorporating detailed discussion on uncertainty and risk analysis.
Response: We agree that additional discussion is desirable, and will expand the discussion of uncertainty analysis in both the Technical Documentation and Users Manual. However it is not the intent of the Technical Documentation to provide extensive background on uncertainty analysis; we will make sure that we provide a reference to such a document.
- Recommendation: Change the positions of some model compartments on Figure 2 of Technical Documentation.
Response: This has already been done.
- Recommendation: Include an index to the technical documentation (repeated under E1 above).
Response: We will consider adding an index or something similar in the future

E3: Comment on the validation reports, including addenda.

Summary of Comments

The responses referred back to B1 and B2.

Recommendations and EPA Responses

None.

Charge Area F: Additional enhancements: What additional enhancements would you recommend to improve the scientific basis or usability of AQUATOX?

Summary of Responses and Recommendations

The reviewers suggested several possible enhancements:

- Recommendation: Develop an option within the Monte Carlo analysis tool to evaluate correlations among variables.
Response: See answer to B3.
- Recommendation: Provide a tool or wizard to facilitate sensitivity analyses.
Response: Sensitivity analysis is available through the Latin Hypercube tool; however it is true that systematically performing sensitivity analyses on all parameters of interest would be tedious and time consuming. Initially we will attempt to provide additional guidance in the users manual and technical documentation with regard to the identifying those parameters most likely to be important. We will investigate other enhancements that could reduce the effort required by the user.
- Recommendation: Perform sensitivity testing of individual parameters to help clarify the accuracy of chemical- and site-specific predictions.
Response: To a large extent sensitivity analysis is an exercise that should be done as part of a site specific model application. This could help guide the user to identify those data which are most important to collect. A systematic, parameter-by-parameter sensitivity analysis of every parameter in AQUATOX would be a huge undertaking.
- Recommendation: Include the ability to draw a food web diagram based on the preference factor matrix and possibly include the option to plot only those trophic links that represent preference factors greater than a user-specified value.
Response: See answer to C7.
- Recommendation: Include features that would maintain a mass balance of nutrients.
Response: 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.
- Recommendation: Include the effects of wave agitation on macrophytes.
Response: see answer to A2.
- Recommendation: Give the user the ability to choose different types of functional responses for consumption.
Response: This is a good suggestion and will be considered for inclusion as a future enhancement, to include functional responses that correspond better to other means of consumption such as filter feeding and raptorial.
- Recommendation: Add the ability to model metals, possibly developing a separate model just for metals.

- Response: see answer to D2

• Recommendation: Provide more validation, especially for additional systems and for mesocosms and where data exist.

Response: see answers to B2 and D1
- Recommendation: Provide experimental studies to support the external concentration to internal concentrations and effects.

Response: see answer to D1
- Recommendation: Add measures of variability to default values.

Response: see answer to C1
- Recommendation: Allow finer time scale simulations.

Response: see answer to A4
- Recommendation: Add 'optimal control' features that allow TMDLs to be calculated.

Response: see answer to D4
- Recommendation: Allow greater spatial disaggregation.

Response: see answers to A2 and A4
- Recommendation: Add segmentation to future versions of *AQUATOX* to improve the ability of the program to model rivers and spatially heterogeneous lakes and reservoirs.

Response: see answer to A2
- Recommendation: Explain that *AQUATOX* is a tool for revealing ecosystem changes that may happen and that it does not make accurate predictions for specific changes in variables, especially indirect effects.

Response: see answer to A2

One reviewer cautioned that the benefits of adding processes should be balanced against the disadvantages of increasing the complexity of *AQUATOX*.

Only one reviewer commented on the ongoing development work. The reviewer feels that the new developments in the model are reasonable.