Report on the Peer Review of AQUATOX Release 3

Executive Summary *(excerpted from final report)*

Reviewers discussed their comments on AQUATOX Release 3 in a series of three teleconferences and submitted final individual comments after these calls. They all agreed 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 one of 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. One reviewer (MM) said it would be useful to "flag" changes to default variables.

While the reviewers agreed that the enhancements to the model were scientifically sound, one reviewer (DP) pointed out that even though the enhancements are consistent with *certain* positions described in the ecological literature, it is not possible for the model to be consistent with *all* of the positions because consistency within the literature does not exist. Two reviewers (MM and DP) said it was hard to measure the model's reasonableness, arguing that its reasonableness depends on its end use. For example, one reviewer (DP) cautioned that "every simplifying assumption used in the model should be known to the user, and it is up to the user to determine the appropriateness (i.e., "reasonableness") of those 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 and is vulnerable to criticism. They stressed the importance of documenting the model's calibration and validation. One reviewer (MM) suggested automating the calibration and validation procedures. Based on the review materials initially provided (a single peer reviewed journal article), the reviewers did not think that the AQUATOX model was sufficiently calibrated or validated. However, additional materials were provided (some of which had been prepared using an earlier version of the model), and these were deemed essential to future users. They recommended that the additional information about the model's calibration and validation be included in the technical documentation. One reviewer (FT) suggested creating an AQUATOX Case Study document to more fully document the verification studies that have been done to date. The reviewers felt that this issue was critical to the model's utility. For example, 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. Two reviewers (MM and FT) said that AQUATOX would be useful for conducting ecological risk assessments as long as the parameters for specific applications are known and there is model validation. Two reviewers (MM and FT) said that AQUATOX could play a role in Total Maximum Daily Load analysis and development, one (FT) qualifying that validation would increase acceptability. The reviewers agreed that the AQUATOX model could be used in conjunction with other tools to identify potential stressors causing impairment of aquatic life. However, one reviewer (FT) cautioned that the model may not be able to distinguish between potential causes if they have the same effects.

The reviewers agreed that while AQUATOX could provide insights into potential effects, it would not be able to establish causal relationships between chemical and physical stressors and their combined, direct, and indirect effects on aquatic biota because several stressors could have similar effects (FT). They also thought that the model was better suited to *supporting* the existing approaches used to develop water quality standards and criteria, as opposed to being used to develop water quality criteria by itself. They noted that the AQUATOX model is one tool among many that should be used in a weight of evidence approach.

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 (MM) commented that the "model enhancements have made AQUATOX one of the most exciting tools in aquatic ecosystem management." Another (DP) 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. One reviewer (FT) pointed out that, from a practical end-use scenario, an unpopular decision can be blamed on the perceived inadequacy of the model, which is not unique to AQUATOX.

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. One reviewer (MM) suggested providing an active link to the documentation for each context-sensitive help file. Another reviewer (FT) recommended retaining the actual User's Manual (i.e., the document that compiles the context-sensitive help files). Also, the reviewer (FT) suggested expanding the tutorial to include some of the enhancements and mentioning it earlier in the User's Manual.

The reviewers thought the sensitivity analysis and tornado diagrams were powerful and useful tools. They recognized the usefulness of the Interspecies Correlation Estimates (ICEs). One reviewer (MM) 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. One reviewer (FT) commented that it "would make a wonderful textbook for an ecotoxicology class." Another reviewer (MM) recommended that the document be divided into

discrete modules to make editing, distributing, and citing easier. To supplement the Technical Documentation and User's Manual, one reviewer (FT) recommended preparing an "AQUATOX Case Study" document to help the user appropriately apply the model to complex situations. A brief summary of each of the sample cases could be included in the notes for each model, and a section in the User's Manual and Case Study document could identify which runs would most likely be informative for specific issues. Also, indicating how long a run might take and providing a list of all the available resources would be useful.

However, now that the model is so user-friendly and accessible, two of the reviewers (MM and DP) 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 (DP) specifically recommended a "user beware" sentence which states that "AQUATOX should only be used (beyond screening purposes only) 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." To help avoid misuse, one reviewer (FT) suggested having live and knowledgeable technical assistance available to answer questions about the model and to assist new users.

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 both the model and the supporting documentation. They agreed that future efforts should focus on model calibration and validation, as well as more explicit documentation where needed. One reviewer (FT) suggested that a future version of the model include metal fate and toxicity, acknowledging that this would be a substantial undertaking. Another reviewer (MM) said that it would be helpful to (1) create default libraries for each third-level ecoregion and reach order/water body type within those ecoregions, and (2) further develop the GIS interface option for stand-alone integration and application, also in a later release. One reviewer (DP) suggested that chemical and organism mass balance be explored, and hyperlinking the original sources to the data inputs. Another reviewer (MM) suggested that it would be useful to be able to simultaneously compare multiple scenarios, and incorporate input range warning flags into the model.