RECENT COMPARISON STUDIES TO ASSIST IN SELECTION OF ADVANCED MODELING TOOLS FOR TMDL DEVELOPMENT

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ABSTRACT

The degree of analysis, and complexity of tools, required to develop TMDL components ranges from simple, screening level approaches based on limited data to detailed investigations driven by extensive data. A variety of interrelated factors determine the analysis approach and tools that are appropriate for developing each TMDL. The factors include the type of impairment, the physical, biological and chemical processes occurring in the waterbody and its watershed; the size of the watershed; the number and type of sources; the amount of time, data and resources available for TMDL development; and the types and costs of actions needed to implement the TMDL. Generally speaking, more detailed and effort-intensive TMDL development techniques are warranted where there is significant uncertainty concerning whether pollutant sources are attributable to human or natural sources and the anticipated cost of controls is especially high. In such situations professionals responsible for TMDL development are likely to be faced with the need to select and use one or more complex, or advanced, environmental simulation models to support their efforts.

This paper focuses on four recent studies performed to compare the capabilities of advanced simulation models. All studies were performed in a research and development context, but all have yielded results that are useful in guiding model selection for TMDL development efforts. Within the TMDL context, models are commonly used to establish the linkage of a variety of water quality targets and sources, and to provide a means for comparing various allocation strategies. The models that were compared in the studies include hydrodynamic, sediment, toxic chemical, eutrophication, bioaccumulation and groundwater models. This paper deals collectively with the materials, conclusions and recommendations that have resulted from the efforts expended in performing recent model comparison studies for the Water Environment Research Foundation (WERF) and the U.S. Environmental Protection Agency Office of Research and Development.

KEYWORDS

TMDL, model selection, water quality models, toxic chemical models, eutrophication models, contaminated sediment models, bioaccumulation models.

GENERAL INTRODUCTION

The use of mathematical models by water quality managers, engineers, and scientists to assess the effectiveness of various control strategies in achieving water use goals and meeting water quality standards has had a long history in the United States. The earliest models were quite simple in nature and were used to address water quality impacts associated with the discharge of pathogens, such as coliform bacteria, and oxygen-demanding materials from large urban areas. With the implementation of the Clean Water Act in the late 1970's and the construction of wastewater treatment facilities, the discharges of pathogens and oxygen-demanding matter from urban areas was significantly reduced. However, this act did not fully alleviate the problems facing our nation's waters. Instead, other pollutants of concern, including nutrients and toxic substances, were identified. To address these new concerns, existing mathematical models were enhanced, and new ones were developed. More recently the U.S. Environmental Protection Agency, together with its counterparts in the state pollution control agencies, has recognized the need to manage point and nonpoint source pollutants on a holistic basis. Models have been required to address an ever-increasing range of pollutants, pollutant fate and transport phenomena, and environmental responses. As a consequence, the number and complexity of mathematical modeling requirements have grown significantly. Often separate models have been developed to evaluate different contaminants and processes, with emphasis on different environmental components (land surface, waterbodies, aquifers).

The transport pathways and fate of naturally occurring constituents, such as solids and nutrients, and contaminants in a watershed are driven by complex interactions of precipitation, land uses, urban and rural watershed runoff, groundwater transport, wastewater and storm water inputs, surface water transport, kinetic transformations and biological processes in the water column and sediment bed. Mathematical models designed to represent the transport pathways and fate of contaminants in the aquatic environment can serve as powerful tools in understanding, and differentiating, the relative significance of natural processes and human activities on trends in water quality and aquatic ecosystem resources. Models can be used to support the development of management plans, such as remediation of contaminated sites or best management plans for agricultural or silvicultural operations, with quantitative evaluations and comparisons of the effectiveness of alternative plans.

In the three decades since passage of the Clean Water Act in 1972, hydrodynamic and water quality models have evolved, in response to both environmental regulations and policies as well as increased performance available from computer technology, from simplified one-dimensional, steady-state models of biochemical oxygen demand and dissolved oxygen to complex two- and three-dimensional, time-varying models of hydrodynamics, carbon and nutrient cycles, eutrophication, aquatic food web dynamics, sediment transport, contaminants transport and fate and contaminant bioaccumulation (Thomann and Mueller, 1987; Chapra, 1997). Water quality models, originally developed to support wasteload allocation studies to determine water quality-based effluent limits for municipal and industrial point source discharges to specific river reaches (USEPA, 1984; 1995), are now applied for watershed-based assessments to determine Total Maximum Daily Loads (TMDLs) for pollutant loads from point sources and nonpoint watershed runoff (Lung, 2001; Lahlou et al., 1998). Coupled with hydrodynamic models, models of sediment transport, contaminant transport and fate, and contaminant bioaccumulation are also used to provide technical input needed for remedial action decisions for the clean-up of contaminated sediments (De Pinto et al., 1994; Tetra Tech, 2000).

Mathematical models are structured as a set of mass balance equations designed to quantitatively represent the key processes and interactions outlined by the conceptual model (i.e., hypotheses) that determine the transport and fate of pollutants, such as organic chemicals or heavy metals, in the aquatic environment. In order to explicitly determine the effect of solids and pollutant inputs from watershed runoff, wastewater discharges and other external sources on transport and fate of the pollutant in the water column and sediment bed, the equations of a model are based on the conservation of mass to properly account for all the inputs, transformations and outflows of the pollutant in the surface water system.

Surface water models are differentiated by the choices made for the definition of the open boundaries of the physical domain and the corresponding specification of terms in the model equations that describe pollutant loads, physical transport processes and kinetic interactions as either (a) externally provided data that are input to the model or (b) internally provided data that are calculated by model formulations. For example, many water quality models define the wetted perimeter and water surface of a water body as the boundaries of the physical domain of the model. Source terms in the model represented by watershed runoff, atmospheric deposition, groundwater interactions and sediment-water exchange of constituents (e.g., nutrients, dissolved oxygen, contaminants) are then provided as externally supplied boundary conditions for input to the model (Imhoff et al., 2003a).

As water quality management issues have become increasingly complex over the past decade, the physical domain boundaries of models have expanded beyond the water column of a water body to explicitly incorporate transport pathways and mass loading of pollutants that are either internally computed or linked with watershed runoff models, regional air quality models, groundwater models, hydrodynamic models, aquatic ecosystem models, sediment diagenesis models, sediment transport and contaminant bioaccumulation models (Thomann, 1998; Di Toro, 2001).

In addition to the choices adopted for the specification of the open boundaries of the physical domain of a model, surface water models are further differentiated by consideration of the spatial and temporal scales of resolution, state variables, kinetic interactions and biogeochemical processes. Collectively these define the level of complexity of a model as: (a) a screening level model; (b) an intermediate level model or (c) an advanced or complex level model.

Screening Models

Screening-level water quality models are designed as highly simplified models to represent only a few selected pollutants as state variables, with limited interactions and few key processes. These models are used to provide preliminary engineering estimates of the effect of pollutant loading on water quality conditions. Analyses using screening models can be performed inexpensively to quickly identify watersheds, geographic areas or river reaches that may have major pollution sources and related water quality problems. EPA's Water Quality Assessment Methodology (WQAM) is an example of a screening level tool that has been applied for relatively simplified calculations of the transport and fate of conventional pollutants and toxic contaminants (Mills et al., 1982).

Intermediate Models

Intermediate, or planning-level, models generally include a more detailed characterization of transport processes and pollutant loads that determine the fate of multiple pollutants, with consideration given to numerous processes and kinetic interactions. Intermediate models often describe a simplified, or "lumped", representation of a state variable (e.g., organic carbon) with no explicit differentiation of either the dissolved and particulate forms or the labile and refractory forms of a constituent. Intermediate models also often describe the mass exchange of a constituent at the sediment-water interface as an externally specified empirical forcing function rather than an internally simulated process. Intermediate models have been developed as one-dimensional, two-dimensional and three-dimensional models, with time dependency of the model represented as either steady-state or time variable. Intermediate models are typically applied to support prioritization and targeting of specific watersheds or river reaches for regulatory control efforts for specific pollution sources, or for comparative evaluations and selection of alternative pollution control strategies to achieve water quality objectives. Examples of intermediate water quality models developed as steady state analytical formulations for assessments of the transport and fate of solids and contaminants in the water column and sediment bed include SMPTOX3 (Limno Tech, 1993) and MICHRIV (USEPA, 1984). Summaries of other intermediate-level formulations for contaminants are given in Dickson et al. (1982).

Advanced Models

Advanced models incorporate state-of-the-art scientific understanding of physical transport and a wide range of aquatic ecosystem processes and kinetic interactions of chemical and biological constituents. Exchange of constituents across trophic levels and between the water column and sediment bed is often represented in complex models to provide a complete mass balance specification of the contaminants of concern. Advanced models, developed originally for research purposes, are now being applied for detailed water quality management and ecological studies of large watersheds (e.g., Chesapeake Bay) and large rivers (e.g., Upper Mississippi River; Middle Hudson River). These models, linked with watershed runoff models and hydrodynamic models, have been developed to address issues related to eutrophication, sediment transport, contaminant fate and bioaccumulation.

Examples of advanced contaminant fate models include CE-QUAL-ICM/TOXI, EFDC, and WASP5-TOXI5. The U.S. Army Corps of Engineers Waterways Experiment Station developed CE-QUAL-ICM/TOXI for eutrophication and contaminant fate studies of nutrient and toxicant loading to Chesapeake Bay (Cerco and Cole, 1993). The contaminant fate model component of EFDC (Hamrick, 1992, 1996; Tetra Tech, 1999a) incorporates kinetic terms for contaminants similar in detail to that used in CE-QUAL-ICM/TOXI, WASP5-TOXI5 (Ambrose et al., 1993) and WASTOX (Connolly and Winfield, 1984). The more advanced contaminant models such as CE-QUAL-ICM/TOXI and EFDC also incorporate advanced sediment transport models (Tetra Tech, 1999b) with state-of-the-art particle deposition and resuspension formulations functionally equivalent to formulations developed for SEDZL, an advanced sediment transport model (Ziegler and Lick, 1986; Ziegler et al., 1990; Ziegler and Nesbit, 1994, 1995).

INTRODUCTION (WERF STUDY)

In order to assist its member subscribers in making the appropriate choice of water quality modeling tools for their specific problems, the Water Environment Research Federation provided funding in 2000 for a study to assess the availability and use of hydrodynamic, runoff, and fate and transport models (Fitzpatrick et al., 2001). AQUA TERRA Consultants teamed with HydroQual and Camp, Dresser and McKee to perform a comprehensive evaluation of currently available models.

Water quality managers and modeling practitioners are often faced with a wide choice of models and modeling frameworks with which to evaluate environmental problems. The purpose of this study was to review the availability and the use of these models. Recognizing that no one model "does it all," the review process segregated models into one or more of the following model classes: rural and urban runoff models, hydrodynamic models, receiving water models for eutrophication and toxic substances, and groundwater models. With the support of the model developers, model descriptions were developed and evaluated with respect to their capabilities and characteristics.

As the project proceeded, the Project Team and WERF participants identified the opportunity to implement the model selection process in the form of an electronic decision making tool. The tool that was developed enables its users to identify, via PC-based interaction, one or more models that are appropriate for an intended application. The decision tool can be used in conjunction with the Final Report for the project to gain further understanding of individual models that appear to offer the most promise as evaluation tools for specific environmental problems.

METHODOLOGY (WERF STUDY)

Model Evaluation

The Project Team made an initial review of the literature and other sources of information concerning mathematical models, including the Internet, and prepared a candidate list of models or computer codes in each of the following five categories:

- Hydrodynamic models – determine the circulation, transport, stratification, and depositional processes within a receiving water,
- Rural and urban runoff models – determine runoff quantity and quality of pollutants,
- Receiving water models – determine the fate and transport of pollutants in surface waters,
- Chemical fate and transport models – a special subclass of receiving water models designed to evaluate toxic chemicals, and
- Groundwater models – determine the fate and transport of pollutants in subsurface soils and porous media and underground aquifers.

The list of candidate models was provided to the WERF Project Manager and Project Subcommittee (PSC) members for their review, in order to ensure that the Project Team did not overlook any candidate models. After a final list of models for evaluation had been identified, a set of evaluation criteria and a standardized evaluation form were established for each model group. Models were characterized in terms of such attributes as media of concern, analysis level(s), methods, temporal representation, dimensional capability, source/release types, sources, assessment extent, applicability to water body types, type of chemicals, critical processes, model uses, resource requirements, model use features, model support, and model availability. Characterizations were developed with an eye towards identifying *distinguishing features* that could be expressed as "decision criteria" that are useful for selecting models within each model class.

Model Selection Tool Development

The second objective of the WERF project was to develop a selection process and criteria for determining the most appropriate model(s) for a particular situation. To satisfy this objective, AQUA TERRA developed a Visual Basic application called the WERF Model Selection Tool.

RESULTS (WERF STUDY)

The study results were made available at no charge to WERF subscribers and for fee to non-subscribers. The final report and the Model Selection Tool were distributed by both CD-ROM and by download from the WERF web site.

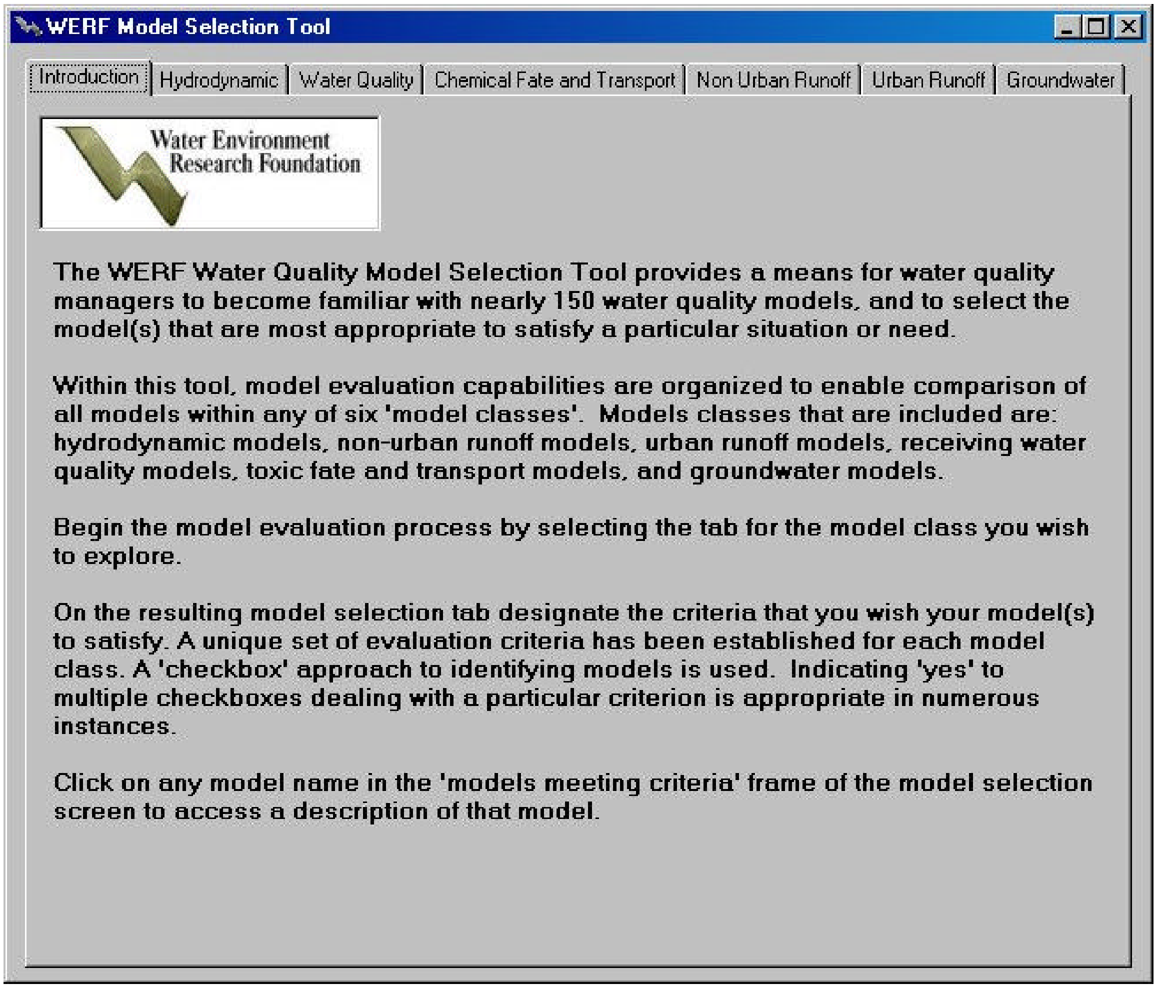
Model Evaluation

The final report for the study included a chapter for each model class that discussed specific considerations for that class, presented a comparison matrix to summarize the results of model evaluation, and provided preliminary guidance on choosing among the models that were evaluated. The model characterization data subsequently served as decision criteria that were built into a computer-based decision tool that enables modelers to interactively evaluate and identify the most suitable model(s) for their intended application.

Model Selection Tool

The WERF Water Quality Model Selection Tool (Figure 1) considers all of the approximately 150 models identified jointly by the Project Team and the WERF PSC.

Figure 1 – Introductory Screen for WERF Model Selection Tool

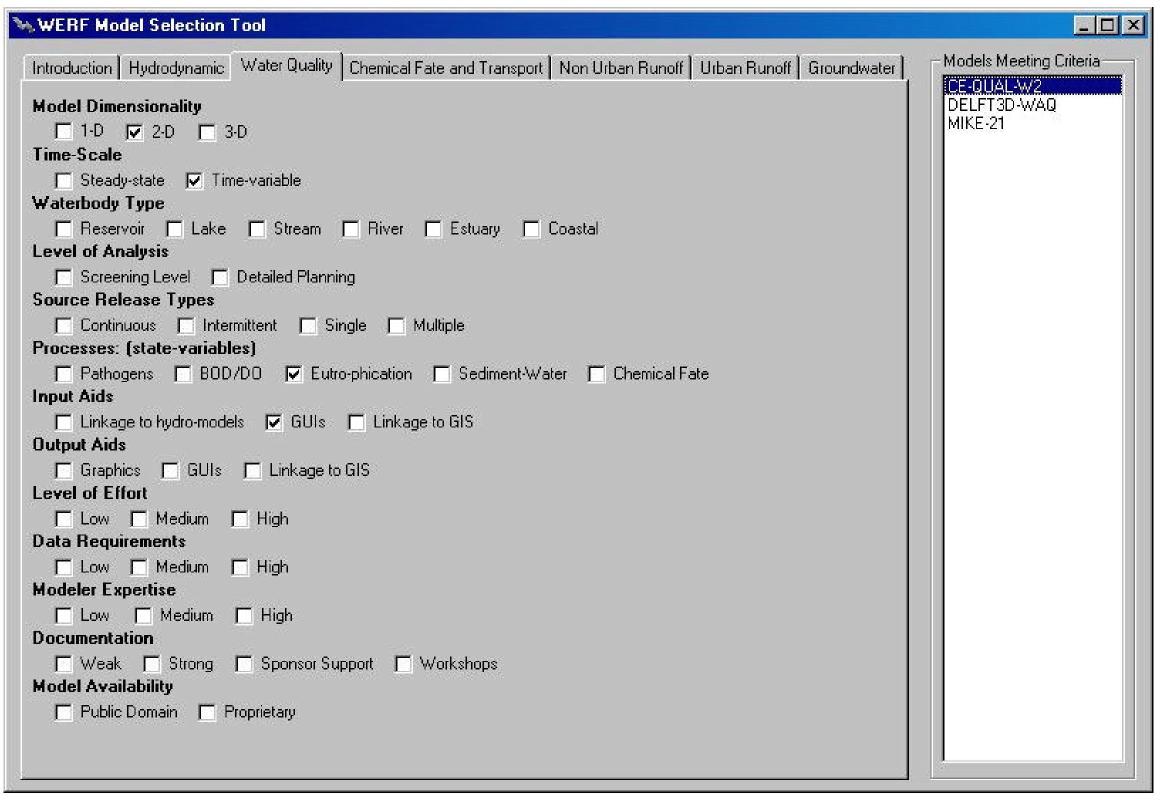


(Fitzpatrick et al., 2001)

Model evaluation capabilities were organized using the previously described model classes; selection criteria, of course, vary somewhat from class to class. A "checkbox" approach was used to help identify the model(s) best suited to the user's needs. That is to say, the user is asked to assign a "yes" or "no" designation to each of the selection criteria used to characterize the models in a particular class. Any checkbox that is left blank is considered as a "no" response. Indicating "yes" to multiple checkboxes dealing with a particular criterion is appropriate in numerous instances. For example, when performing a search within the receiving water quality model class, checking the boxes indicating a capability to perform both "1-D" and "2-D" computations may be appropriate if the modeler is looking for a single model with which he/she might perform first a screening-level analysis, and subsequently a more detailed analysis.

As the checkbox designations are made, the tool continually updates a list of models that satisfy the requirements indicated by the user. By either tightening or loosening the model requirements, the user is able to identify an appropriate number of models for more detailed consideration. Model descriptions are available within the decision tool for all models; a user is able to access the description for any model by clicking on the model name in the "models meeting criteria" frame of the model selection screen (Figure 2). These model descriptions provide an initial source for additional information, and at the same time provide guidance on how to obtain technical assistance and/or more detailed documentation.

Figure 2 – Example Screen for Selecting a Water Quality Model.

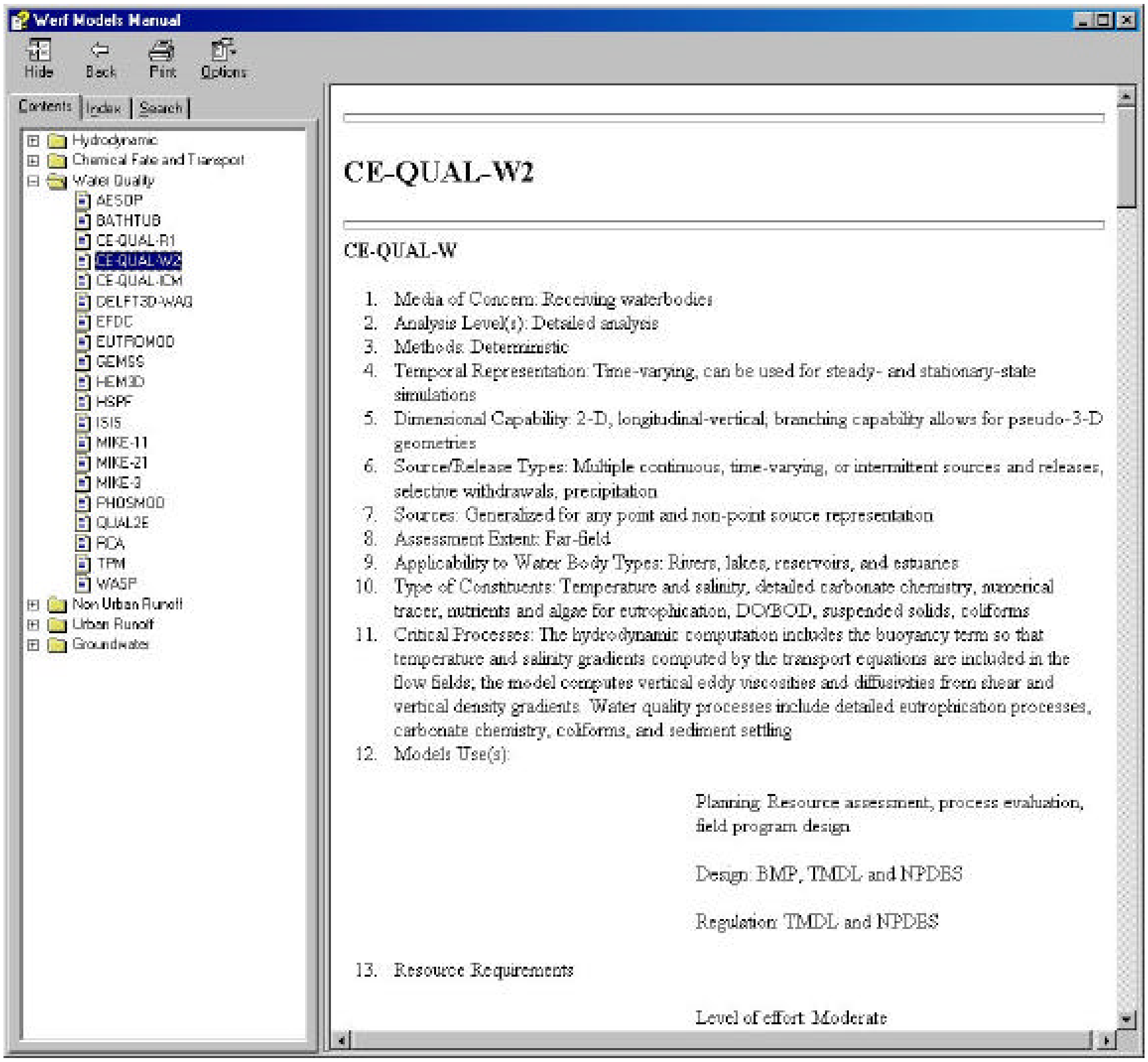


(Fitzpatrick et al., 2001)

Figure 3 provides a sample model description for CE-QUAL-W2 (Cole and Buchak, 1995) that demonstrates the type and level of detail of the supporting information that is available for each model included in the selection tool.

The WERF Water Quality Model Selection Tool has been implemented using Visual Basic for specification of the user interface, an Access database for storage of search criteria and a compiled HTML help file for storage of detailed information about models and web links. The model classes and related selection criteria are stored in the Access database. The user interaction screens are generated at run time from the information in the database. This makes it easy to refine criteria over time. The detailed information about the models stored in the compiled HTML help file has extensive search capabilities in its own right. User's can search for any term appearing in any model description.

Figure 3 – Example Screen Showing Detailed Data for a Selected Model (CE-QUAL-W2)



(Fitzpatrick et al., 2001)

CONCLUSIONS (WERF STUDY)

Recent follow-up conversations with the WERF Project Manager for this effort (Moeller, 2003) suggest that the study results were considered successful, and that dissemination of the results has been significant. Based on records maintained at WERF, 192 copies of the study results during the past two years have been distributed to date, with the following distribution breakdown:

- WEF (CD-ROM): 48

- WERF Subscribers (CD-ROM): 81
- WERF Subscribers (electronic download): 63

WERF has discussed and presented the study in numerous presentations, and has received favorable responses from its subscribers and others. It is WERF's intention to periodically update and expand both the model evaluations and the Model Selection Tool. As an element of this update, WERF may solicit additional feedback from users on the utility of the study results, as well as suggestions for improvements.

WERF is currently involved in outreach to state permitting authorities to make them aware of the Model Selection Tool, as well as other WERF research on models and modeling systems.

INTRODUCTION (EPA STUDIES)

The WERF study was preceded and followed by highly detailed model comparison studies funded by EPA Office of Research and Development. The first study in 1999 compared advanced eutrophication models, and two subsequent studies compared contaminated sediment models in 2002, and chemical bioaccumulation models in 2003.

Eutrophication Model Evaluation

EPA's Office of Research (ORD) is taking an active role in supporting the States' needs for modeling tools useful for TMDL development. Within ORD considerable efforts are in progress related to improving, and facilitating the use of, models for watershed loadings, receiving water quality and ecology. In 1999, ORD's Ecosystem Research Division in Athens, Georgia funded HydroGeoLogic and AQUA TERRA Consultants to evaluate and compare receiving water models useful for developing nutrient TMDLs that require vigorous characterization and understanding of environmental conditions and response (HydroGeoLogic, 1999). Dynamic modeling tools appropriate for developing TMDLs for different environmental settings, with a broad range of dimensional and hydrodynamic complexity were considered. While the focus of the study was on water column models, the evaluation also encompassed a consideration of the relationship of these models to bed sediment models, ecological models, and watershed loadings models.

It was a goal of the study to focus the majority of the effort on performing a meaningful head-to-head evaluation of a small number of the most promising models. To accomplish this goal, the Study Team established, and applied, a set of screening criteria to the available models to identify those models that offered superior features and warranted detailed evaluation. Minimum requirements were established as follows:

- Models must embody a well-developed representation of receiving water quality processes that enables detailed simulation of sediment, nutrients and plankton.
- Water quality/eutrophication models must either be internally linked to a hydrodynamic model, or have been successfully coupled externally to a

hydrodynamic model. Internally- or externally-linked hydrodynamic models must be dynamic.

- Models must have adequate documentation that explains what the model does and what algorithms it uses; operational instructions were also a requirement.
- Support must be readily available for models; for more complex models, it was not a requirement that the support be provided without fee.
- Models must have been used in a minimum of three applications during the last ten years, with at least one application performed by a party other than the developer or the developer's immediate work associates.
- The model code must either be non-proprietary, or it must be possible to make a one-time purchase of the code and documentation without a run-time licensing requirement. For less complex models source code must be obtainable; for more complex models in lieu of source code, executable code must be obtainable.
- For reservoir and estuary models, the model must be multi-dimensional. One-dimensional models were not considered.

A small number of models (seven) were identified that were judged superior to all others in their promise as tools for eutrophication analysis over a broad range of water body environments. Given practical considerations, a model's superiority was determined not only by its scientific and operational features, but by issues such as model availability, model support, and application experience. These models were then compared and characterized in detail. In addition, the models' potential for linkage to a comprehensive watershed loadings model was evaluated.

Contaminated Sediment Model Evaluation

EPA ORD is also currently supporting EPA's Office of Emergency Response and Remediation (OERR) by addressing priority research needs related to assessing the fate and transport of pollutants via contaminated sediment and bioaccumulation. To this end, EPA ORD's National Exposure Research Laboratory is once again providing support through its Ecosystem Research Division (ERD) in Athens, Georgia. To begin the support effort, an initial project was formulated by ERD in 2002 and completed by AQUA TERRA and its consultants Dynamic Solutions and J.E. Edinger Associates in early 2003 (Imhoff et al., 2003a). The objective of the study was to perform an evaluation of currently available numerical models usable for assessing fate and transport of contaminated sediments. At the onset of the study ERD established a list of attributes that each model must possess. These included:

- Models must represent state variables and physiochemical processes that affect the fate and transport of sediments and contaminants.
- Model code must either be non-proprietary, or it must be possible to purchase the code and supporting documentation without a run-time licensing requirement.
- Contaminated sediment model must have either an internal linkage or external coupling to a hydrodynamic model.
- Model support must be available, including adequate, up-to-date documentation/user manual.

- Model must have an adequate history of application.
- Model must be amenable to linkage with a watershed model.

The Study Team performed the model evaluation study within the constraints described above. In considering ERD's needs, we made additional refinements to the scope that better define the modeling components and the range of model complexity that were evaluated. To provide ERD with a basis on which to compare the best models and select one or more as the "chassis" into which model enhancements may be built, a head-to-head comparison of the models was developed applying a high level of scrutiny to both model science and model usability. Finally, the study considered the issues and strategies involved in linkage of the contaminated sediment models to a comprehensive watershed model.

Bioaccumulation Model Evaluation

A parallel model evaluation for chemical bioaccumulation models is currently being performed by AQUA TERRA with the assistance of Eco Modeling and Dynamic Solutions (Imhoff et al., 2003b). ERD required similar attributes for the bioaccumulation models that were to be evaluated:

- Models must represent state variables and physiochemical processes that determine the phenomena of bioaccumulation and biomagnification of chemicals within biotic food chains.
- Model code must either be non-proprietary, or it must be possible to purchase the code and supporting documentation without a run-time licensing requirement.
- Model support must be available, including adequate, current documentation/user manual.
- Model must have an adequate history of application.
- Model must be amenable to linkage with models that have been developed for related environmental media compartments.

For the current effort the Study Team is evaluating dynamic bioaccumulation models, including food chain, food web, population, and pharmacokinetic models, that represent uptake and clearance of organic chemicals, metals, and radionuclides; bioavailability of a chemical is considered critical. Key attributes are being evaluated for comparing constructs contained in a bioaccumulation model and in supporting models for chemical fate and transport, chemical equilibrium, sediment geochemistry (for metals), and toxicity.

In all three EPA studies AQUA TERRA and its partner firms investigated and evaluated the best of the current generation of advanced models for receiving waters. The three studies followed a parallel approach, and resulted in comparison of models at a level of detail not previously performed or documented.

The cornerstone of the studies was identifying a small number of the best intermediate and advanced models or model compartments for detailed comparison. Each of the studies included a consideration of linkage issues between the environmental modeling compartment on which the study was focused and models for one or more adjoining environmental media. The eutrophication study and the contaminated sediment study considered issues and strategies related to linking the studies' models to watershed loadings models. The bioaccumulation study will consider issues related to linking the subject models to models representing a handful of adjoining environmental compartments. The recommendations developed in all three studies were specific to ERD's needs for identifying and potentially enhancing intermediate and advanced environmental models. However, the results obtained by performing the detailed model comparisons were of value to a broader audience that includes professionals involved in TMDL development. The approach used to document the models which were compared in detail varied from study to study, but the final reports for all three studies provide in-depth information on the selected models that is presented at a level of detail that is highly useful for supporting the selection of one or more models for use within a TMDL context.

METHODOLOGY (EPA STUDIES)

The methodology used to develop each of the three EPA studies was similar, with the initial evaluation of eutrophication models providing the conceptual template for the subsequent studies (Figure 4). All three studies included the following tasks:

- Developing evaluation criteria
- Identifying candidate models
- Performing model screening
- Performing detailed model evaluations
- Evaluating model linkage issues
- Developing recommendations
- Documenting models

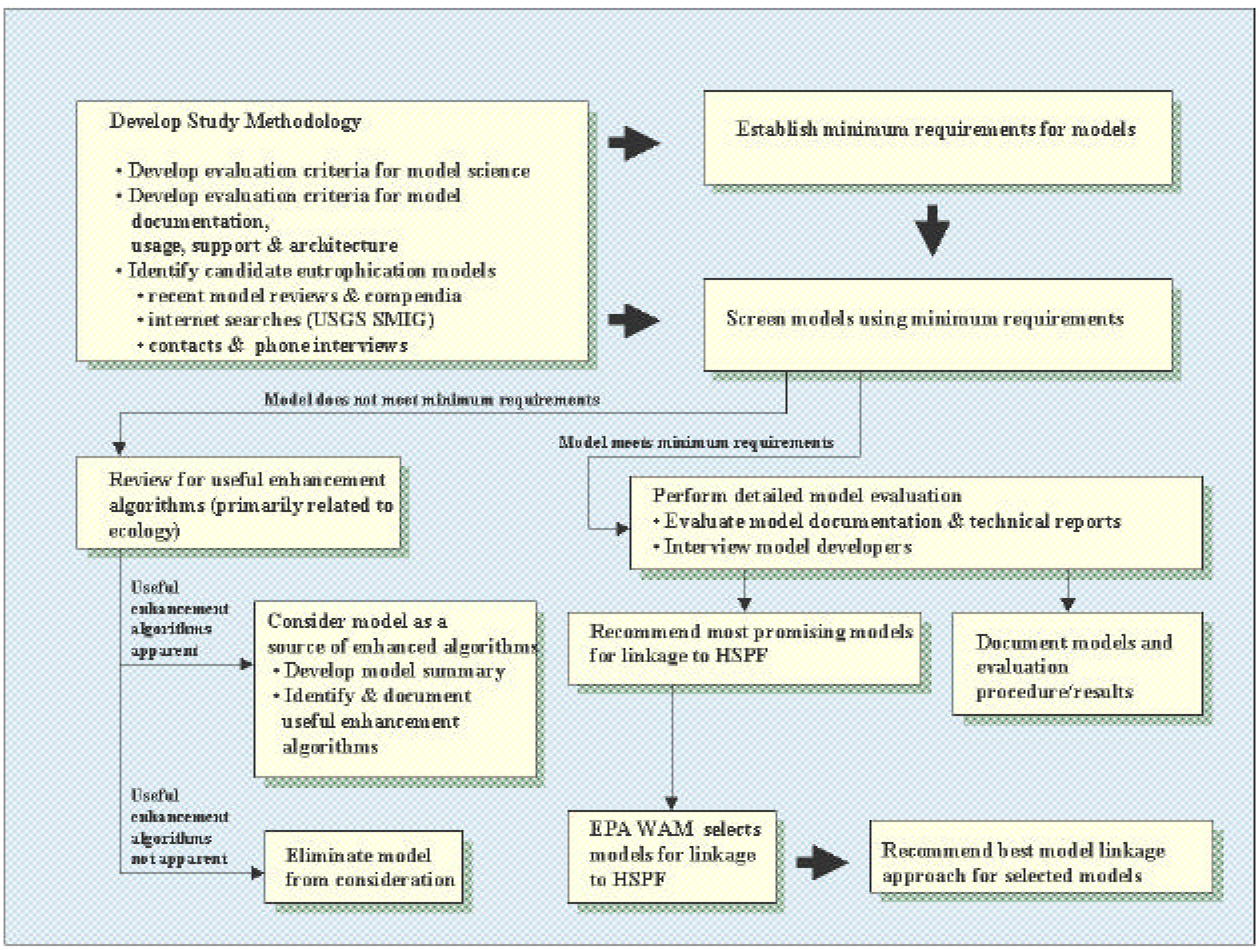
Developing Evaluation Criteria

Two tiers of evaluation criteria were developed. First-tier, or screening, criteria were established to identify the models or modeling components that offer ERD the most advantage as tools for carrying out a variety of model research and development activities. Second-tier, or comparison, criteria were established to develop a basis for detailed head-to-head comparison of models satisfying all screening requirements. Both model science and model support and usability features were considered. In each of the three studies, modeling capabilities for multiple environmental compartments were considered. The 1999 eutrophication model evaluation placed its emphasis on comparing eutrophication state variables and processes, but considered hydrodynamics, sediment transport, bed sediment and ecological processes as well. To fully address contaminated sediment issues, the Study Team for the second evaluation in 2002 concluded that four modeling components needed to be considered: hydrodynamic models, sediment transport models, toxic chemical transport and fate models, and conventional pollutant transport and fate models. Both tiers of criteria were customized to address the specific capabilities of each of the component groups. The Study Team for the ongoing bioaccumulation model evaluation is focused on characterizing bioaccumulation and bioavailability state variables and processes, but is also considering capabilities that the selected models exhibit for chemical fate and transport, chemical equilibrium, sediment geochemistry (for metals), and toxicity.

Identifying Candidate Models

For each of the three studies, recent model reviews and compendia were used to identify many of the currently available models. Additional models were identified through personal knowledge of the Study Team participants; by means of phone calls to knowledgeable professionals; and by investigating a comprehensive set of internet links provided on the USGS Surface-water quality and flow Modeling Interest Group (SMIG) web page, as well as other Internet-based resources.

Figure 4 – Study Methodology for 1999 EPA ORD Comparison of Eutrophication Models for Use in TMDL Studies.



(HydroGeoLogic, 1999)

Performing Model Screening

First-tier criteria were applied to the list of candidate models to perform a preliminary screening. For the contaminated sediment model study a unique set of screening criteria were applied to each of the four modeling components that determine contaminated sediment transport and fate. The Study Team further scrutinized the remaining models; using additional information gained by discussions with the model developers, the Study Team and the EPA Work Assignment Manager eliminated additional modeling components. For the eutrophication model study, seven models passed the screening and were evaluated in detail. The screening resulted in selecting five hydrodynamic models, six sediment models, six toxic chemical models, and five conventional pollutant models for detailed evaluation and comparison in the contaminated sediment study. Eight models passed the screening performed for the bioaccumulation model study.

Performing Detailed Model Evaluation

The models that survived the screening effort were further evaluated by applying a more vigorous and comprehensive set of comparison criteria. To perform the model science evaluation, the second-tier, or comparison, criteria that had been established at the beginning of each study were translated and expanded into tables that compared the models included in each of the component groups on a state variable by state variable and process by process level. In addition, the screening-level assessment of model support and usability was expanded to evaluate availability and general quality of documentation; availability of application aids such as graphical user interfaces, and pre- and post-processors intended to enhance ease-of-use; availability of Ahuman support@ in the forms of developer/sponsor assistance, user=s groups, workshops, web sites, and conferences/symposia; and the characteristics of model usage (application history and application resource requirements).

Evaluating Model Linkage Issues

For the eutrophication model study, the linkage analysis included the following elements:

- Description of a loose coupling strategy with model interaction controlled by ‘watershed supervisor’ software
- Definition of watershed supervisor tools and functions
- Discussion of linkage issues related to the proposed coupling strategy
- Characterization of HSPF (Bicknell et al., 2001) watershed model operations and outputs as they are relevant to linkage
- Identification of linkage issues unique to each of the selected receiving water eutrophication models

For the contaminated sediment model study, the Study Team investigated issues involved in linking the models that were evaluated in detail to a comprehensive watershed model. The issues involved in linking watershed and waterbody models were identified and discussed. A generic information exchange mechanism was formulated and described that would mediate the coupling between any two models. This approach simplifies the investigation, and later implementation, of coupling between all possible pairs of models. Various issues involved in watershed-waterbody model linkage were discussed and criteria for evaluation were distilled. A preliminary narrative evaluation of compatibility with such a linkage approach was performed for several waterbody models.

The model linkage analysis for the bioaccumulation model study has not yet been formulated or performed.

Developing Recommendations

The Study Team developed recommendations regarding the most promising models for use in achieving ERD's potential model enhancement and application activities. In making recommendations both science and non-science criteria were considered. Final recommendations were based on qualitative, composite model comparisons.

Documenting Models

Summary documentation was developed for each model for which detailed evaluation was performed. The information needed to characterize the models was obtained from user=s manuals, technical papers, other model evaluations, and personal contact with model developers or support groups.

RESULTS (EPA STUDIES)

Figure 5 provides a composite view of all models for which detailed evaluation was performed within the context of the three model evaluation studies funded by EPA. Collectively, modeling capabilities for five environmental compartments were compared in detail:

- Hydrodynamics
- Sediment transport
- Toxic chemical transport and fate
- Conventional pollutant transport and fate and eutrophication
- Chemical bioaccumulation

In some cases, a model with more limited scientific scope was evaluated within the context of a single environmental compartment. Models with a broader scope of modeling capabilities, such as EFDC (Hamrick, 1992), were evaluated within the context of more than one compartment.

To provide EPA ERD with a basis on which to compare these models and select one or more as the "chassis" into which model enhancements may be built, a head-to-head comparison of the models was developed applying a high level of scrutiny to both model science and model usability. The capabilities and scope of models were compared on a state variable-by-state variable and process-by-process basis. Figure 6 provides an example of the level of detail used for characterizing the state variables included in the conventional pollutant transport and fate models, and Figure 7 provides an example of the level of detail used for comparing the scientific processes included in models for sediment transport. (The complete tables extend past the length of the examples given.) Viewed as a whole, the comparison of intermediate and advanced models that has been carried out to date encompasses the following breadth:

- Hydrodynamic models: **5** models were characterized in terms of **19** state variables and **54** processes, features and approximations.
- Sediment transport models: **6** models were characterized in terms of **12** state variables and **53** processes.
- Toxic chemical transport and fate models: **6** models were characterized in terms of **5** state variables and **37** processes.
- Conventional pollutant fate and transport models: **9** models were characterized in terms of **45** state variables and **106** processes.

The full extent of state variables and processes that will be used to characterize the bioaccumulation models is presently under development.

Figure 5 – Models Selected for Detailed Comparison in Recent EPA ORD NERL ERD Evaluations.

Figure 6 - Example of the Level of Detail Used for Comparing the State Variables for the Conventional Pollutant Transport and Fate Models.

Table 3.4. Comparison of Conventional Pollutant Transport and Fate Model State Variables

	AQUATOX V.2.0	CE-QUAL-ICM V.1	EFDC	HSPF-RCHRES V.12	WASP5(6)-EUTRO5(6)
Plankton					
Single, Generalized Water Column Algae Compartment				★	★
Multiple Water Column Algae Compartments	★	★	★		
Single, Generalized Benthic Algae Compartment			★		
Multiple Benthic Algae Compartments	★			7	
Single, Generalized Zooplankton Compartment				★	
Multiple Zooplankton Compartments	★				
Other Biota					
Macrophytes	5			3	
Animals	6				
Pathogens as Generalized Decaying Substance				★	
Pathogens as Fecal Coliform Bacteria			★		4
Nitrogen					
Ammonium				★	
Dissolved Ammonia				★	
Total Dissolved Ammonia/Ammonium	★	★	★	★	★
Ammonia Adsorbed to Inorganic Sediment				★	
Nitrate + Nitrite	★	★	★	★	★
Total Organic Nitrogen					★
Dissolved Organic Nitrogen		★	★		1
Particulate Organic Nitrogen					1
Labile Particulate Organic Nitrogen		★	★	2	
Refractory Particulate Organic Nitrogen		★	★	★	
Phosphorus					
Dissolved Inorganic Phosphorus	★	★	★	★	1
Phosphate Adsorbed to Inorganic Sediment		★	★	★	1
Total Organic Phosphorus					★
Dissolved Organic Phosphorus		★	★		1
Particulate Organic Phosphorus					1
Labile Particulate Organic Phosphorus		★	★	2	
Refractory Particulate Organic Phosphorus		★	★	★	

footnotes

1 Organic N, organic P, CBOD, ammonia and phosphate may each be divided into dissolved and particulate fractions by a different time-constant but spatially variable user-defined fraction. Only the total concentration of each is tracked as a state variable, and all interactions except settling apply to the total. The settling rate is also input by the user, but may be both spatially and temporally variable. There are two effects of defining the partition between dissolved and particulate forms. The effective settling rate is modified and the algal growth rate limiting factor is affected since it is based on the concentration of the dissolved form of nutrients.

2 Labile particulate organics are modeled as CBOD.

3 One of multiple benthic algae compartments can be used to model macrophytes.

4 Coliforms are not a state variable in WASP5, but are a state variable in WASP 6.1.

5 AQUATOX has multiple macrophyte compartments including byrophytes.

6 AQUATOX has multiple animal compartments including aquatic insects, mollusks, size and age classes of fish.

7 Multiple benthic algae compartments are an undocumented feature of Version 12.

(Imhoff et al., 2003a)

Figure 7 - Example of the Level of Detail Used for Comparing the Model Processes for the Sediment Transport Models.

Table 3.2. Sediment Transport Model Processes

	ECOMSED V.1.3 & SEDZL .	EFDC & EFDC1D V.1	HSCTM-2D V.1	HSPF-RCHRES V. 12	IPX 2.7.4	WASP5(6)-TOXI5(6)
SUSPENDED LOAD TRANSPORT (COHESIVE & NON-COHESIVE SOLIDS)						
Cohesive Solids (silts, clays, POM, <63 micron grain size)						
Settling/Deposition/Resuspension Provided as Input					★	★
Settling/Deposition/Resuspension Computed Internally	★	★	★	★		
Flocculation						
Not Represented				★	★	★
Explicit Flocculation Model						
Implicitly Accounted for in Settling Velocity Function	★	★	★			
Settling Velocity						
Settling Velocity Provided as Input	★		★	★	★	★
Accounts for Hindered Settling as f(high suspended sediment concentration)		★	★			
Accounts for Free/Discrete Settling as f(size class)		★	★	★		
Accounts for Organic Matter Content of Suspended Matter						
Resuspension						
Resuspension Velocity Provided as Input					★	★
Calculated as Function of Bed Bulk Density & Critical Shear Stress or Bed Shear Strength	★	★	★	1		
Accounts for Effect of Bed Armoring	★	★				
Accounts for Organic Matter Content in Bed						
Deposition						
Deposition Velocity Provided as Input	★			★	★	★
Calculated as a Function of the Bottom Layer Velocity/Bed Stress	★	★	★			
Accounts for Composition of Sediment Flocs in Predicting Deposition Rate						
Non-Cohesive Solids (sands, >63 microns grain size)						
Settling/Deposition/Resuspension Provided as Input					★	★
Settling/Deposition/Resuspension Computed Internally	★	★				
Carrying Capacity Computed Internally	★			★		
Settling Velocity						
Settling Velocity Provided as Input	★				★	★
Accounts for Hindered Settling as Function of High Suspended Sediment Concentration		★		★		
Accounts for Free/Discrete Settling as Function of Particle Size	★	★				
Resuspension						
Resuspension Velocity Provided as Input					★	★
Calculated as Function of Bed Bulk Density & Critical Shear Stress or Bed Shear Strength	★	★				
Accounts for Effect of Bed Armoring	★	★				
Deposition						
Deposition Velocity Provided as Input					★	★
Calculated as a Function of the Bottom Layer Velocity/Bed Stress	★	★				
Wave Current Interaction on Bed Shear Stress						
Not Represented			★	★	★	★
Represented	★	★				
BED LOAD TRANSPORT (NON-COHESIVE SOLIDS)						
Not represented	★		★	★	★	★
Rates Computed Internally		★				

footnotes

1 influence of bed composition on resuspension represented as input 'erodibility' factor

(Imhoff et al., 2003a)

CONCLUSIONS (EPA STUDIES)

Within the context of meeting EPA Ecosystem Research Division's objectives, the model evaluation studies appear to be on track. The eutrophication study results have been presented to several audiences as one of the Agency's research and development products to support the States in carrying out the TMDL process. The results of the contaminated sediment model evaluation have been distributed to seminar attendees of at EPA's Office of Emergency Response and Remediation, to the members of EPA's Contaminated Sediment Technical Advisory Group (CSTAG), and to EPA Regions.

As the final component of the model evaluations, the EPA Work Assignment Manager intends to apply a number of the high ranked models (from both the contaminated sediment and the bioaccumulation model evaluations) to different types of surface waters, ranging from a relatively small Piedmont river to a salt-wedge estuary.

The study results also offer a unique opportunity to a broader audience of professionals who have a need to select advanced modeling tools to support TMDL studies. Generally speaking, the more detailed and effort-intensive TMDLs that require and use advanced modeling tools do so because there is significant uncertainty concerning whether pollutant sources are attributable to human or natural sources. Resolving this uncertainty is contingent on using a model that provides a robust consideration of the dominant physical, chemical and biological processes that dominate the waterbody for which a TMDL is being developed. To the extent that a model does not represent one or more processes that dominate the fate of a pollutant of concern for a specific waterbody, the model's results can compound uncertainty, rather than eliminate it. The three model evaluation studies for EPA described above provide a characterization of the most promising advanced environmental models at a level of detail that has not been previously documented. The study results enable a knowledgeable professional to identify and evaluate the unique strengths of the science contained in each of the models. By doing so, they offer an opportunity to determine a more comprehensive match between model science and the setting in which the model is to be applied. Undoubtedly other considerations will come into play in selecting the model that will eventually be applied; nonetheless it is always preferable to gain the fullest possible understanding of the strengths and weaknesses of a model prior to the modeling effort, rather than during or after the modeling effort.

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