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# EVALUATION OF CONTAMINATED SEDIMENT FATE AND TRANSPORT MODELS
# FINAL REPORT

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## ABSTRACT

EPA's Office of Research and Development (ORD), National Environmental Research Laboratory (NERL), Ecosystem Research Division (ERD), is 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. ORD has proposed projects for funding by OERR that include a broad range of model evaluation, development and application activities and products. The work effort described in this report constitutes the first element of the support effort by ERD. The study provides an evaluation of currently available numerical models useful for assessing fate and transport of contaminated sediments. By means of an objective and reproducible process a small number of models are identified that are judged superior to all others in their promise as tools for contaminated sediment analysis over a broad range of water body environments. To provide 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 is developed applying a high level of scrutiny to both model science and model usability. Finally, the study considers the issues and strategies involved in linkage of the contaminated sediment models to a comprehensive watershed model.

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Accurate evaluation of many of the complex models included in this study was aided by model developers who made themselves available to answer questions and review our preliminary conclusions. Among those who deserve a special thanks for participating in this process asre Dr. Richard Park (Eco Modeling, Inc.), Dr. John Hamrick (Tetra Tech, Inc.), Dr. Carl Cerco (US Army Corps of Engineers), Mr. James Fitzpatrick (HydroQual, Inc.), Dr. Kirk Ziegler (QEA), and Dr. Mark Dortch (US Army Corps of Engineers).

Among the authors, Mr. John Imhoff was the Work Assignment Leader/Manager for AQUA TERRA. Mr. Imhoff designed the study methodology and coordinated the communications between the study's participants as the methodology was carried out. He had primary responsibility for developing the study reports and assuring that QA/QC was performed effectively throughout the study. Dr. Andrew Stoddard of Dynamic Solutions, Inc. was instrumental in defining/refining the first-tier criteria that were applied to screen candidate models, and the second-tier criteria that were used to compare the models that underwent detailed evaluation. He also developed the descriptive materials for the various modeling component groups and provided conclusions and summary materials related to the detailed model comparisons. Mr. Edward Buchak of J.E. Edinger Associates provided input and review for all aspects of the study and directed the efforts of his firm's staff.

Mr. Paul Duda of AQUA TERRA coordinated the screening effort that identified the models subsequently included in the study's detailed comparisons. Mr. Anthony Donigian, Jr. served as AQUA TERRA's Technical Monitor for this Work Assignment; in this capacity he performed numerous technical reviews to assure the quality, consistency and completeness of the final product.

Dr. George Krallis of J.E. Edinger Associates evaluated model support and usability issues, and developed the discussion of these issues that is included in the Final Report. Dr. Rajeev Jain of J.E. Edinger Associates performed and reported the issues related to linking contaminated sediment receiving water models to watershed models.

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# EXECUTIVE SUMMARY

## Introduction

This study provides an evaluation of currently available numerical models useful for assessing fate and transport of contaminated sediments. By means of an objective and reproducible process a small number of models are identified that are judged superior to all others in their promise as tools for contaminated sediment 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. At the onset of the study ERD established a list of attributes that each model must possess. These include:

- 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 that were, and were not, evaluated; and the range of model complexity that was, and was not, 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 considers the issues and strategies involved in linkage of the contaminated sediment models to a comprehensive watershed model.

## Study Methodology

The Study Team developed and carried out a methodology that was comprised of the following elements:

- <u>Developing evaluation criteria.</u> Two tiers of evaluation criteria were developed. First-tier, or screening, criteria were established to identify the contaminated sediment 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. To fully address contaminated sediment issues, the Study Team concluded that four modeling components must 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.

- Identifying candidate models. Recent model reviews and compendia were used to identify many of the currently available tools for modeling contaminated sediment in receiving waters. 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. In establishing the list for screening, the models were not required to embody more than one of the four contaminated sediment modeling components. A list of approximately 120 models, or modeling components, was identified.

- Performing model screening. The first-tier criteria were applied to the list of candidate models to perform a preliminary screening. 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 Work Assignment Manager eliminated additional modeling components. 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.

- 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 the 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. 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.

- Developing recommendations. The Study Team developed recommendations regarding the most promising models for use in achieving ERD’s planned contaminated sediment 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.

- <u>Documenting models.</u> 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.

**Conclusions and Recommendations**

The study resulted in conclusions and recommendations regarding model science; model support, usage and usability; and model linkage issues and strategies.

<u>Model Science</u>

(1) Prior to initiating the development of any model for a site-specific contaminated sediment problem, it is essential that a 'conceptual model' be prepared to help guide the model selection process. The 'conceptual model', based on an inventory, compilation and analysis of the available site-specific data, identifies the most significant physical, biological and geochemical processes and interactions that control the transport and fate of solids and the toxicant(s) of concern. Of critical importance for the development of a site-specific model, the 'conceptual model' identifies the availability of data as well as any critical data gaps. In addition to the scientific data and information gathered, the 'conceptual model' clearly identifies the state, local or federal regulatory issues and/or resource management issues related to the contaminant of concern. The 'conceptual model' clarifies the purpose/objectives/goals of the intended contaminated sediment modeling study. Finally, the 'conceptual model' serves to identify the level of scientific detail required to support the decision-making process. The availability of site-specific data, the level of scientific detail required for scientifically defensible decision-making, and the availability of skilled personnel and the resources allocated for the study, in turn, all enter into the selection of either intermediate level model(s) or advanced level model(s) for the contaminated sediment modeling framework.

(2) The state of scientific knowledge incorporated in the advanced versions of hydrodynamic models, sediment transport models, toxic chemical transport and fate models and conventional pollutant models is at a very impressive level of detail. The representation of specific processes can usually be improved. In all the models evaluated, however, one missing link stands out. Organic matter generated by biological models is not internally coupled with either sediment transport models or toxic chemical models. Distributions of dissolved (DOC) and particulate organic carbon (POC) that are needed for three-phase partition calculations in a toxic chemical model are empirically assigned as input data to parameterize the distributions of DOC and POC in the following toxics models: EFDC, EFDC1D, WASP-TOXI and IPX.

(3) User-assigned settling velocities are used to parameterize the settling and deposition of algae and particulate organic carbon (POC) in biological models. A more rigorous approach would be to internally couple the sediment transport formulations used for deposition and resuspension of cohesive solids to describe settling, deposition and resuspension of biologically simulated algae and POC in the water column and bed.

(4) With the exception of AQUATOX, dissolved (DOC) and particulate organic carbon (POC) in the water column and bed generated by a biological model are not internally coupled with the

organic carbon-based three-phase partitioning model used in toxic chemical models. User-assigned distributions of POC or fractions of organic carbon (Foc) are combined with solids simulated by the sediment transport model to parameterize POC in the water column and bed. User-assigned distributions of DOC are input to describe DOC in the water column and bed. A more rigorous approach would be to internally couple biologically simulated water column and bed DOC and POC with the three-phase partition calculations in a toxics model.

(5) Internal coupling of a biological model with sediment transport and toxic chemical models would, by eliminating the need for user-assigned parameterization of algae and POC settling rates, and distributions of POC and DOC, decrease the degrees of freedom presently allowed in the mass balance models for sediment transport, toxic chemicals and eutrophication.

(6) The present approach for toxic chemical models, dependent on the modeler's parameterization of DOC/POC distributions and the fraction of organic carbon in the water column and bed, has been applied in numerous toxic chemical modeling studies over the past two decades. There are three key assumptions, implicit in the 'conceptual model' for these studies, that justify the empirical parameterization of organic carbon data as input to a toxics model. The assumptions are: (1) seasonal/spatial patterns of biological production can be reliably described by repeatable patterns; (2) biologically produced organic matter is a minor component of the total solids budget; and (3) remediation alternatives are not expected to alter seasonal/spatial patterns of biological production.

(7) If these key assumptions are not supported by the site-specific 'conceptual model' then a biological model should be internally coupled with the sediment transport and toxic chemical models to properly describe the interaction of DOC and POC with the three-phase partition calculations of the toxics model.

(8) If there is a need to couple a biological model with a sediment transport model and a toxic chemical model to build a credible contaminated sediment model framework, the selection of an intermediate biological model (e.g., WASP-EUTRO) could provide an appropriate level of biological detail rather than a more complex advanced biological model (e.g., EFDC or CE-QUAL-ICM).

(9) Of all the intermediate and advanced models evaluated for this study, implementation of these recommendations would be the most straightforward in EFDC. The EFDC model framework includes a toxics model and an advanced water quality/eutrophication model that is coupled with the hydrodynamics and sediment transport models. These recommendations could also be implemented in AQUATOX since the sediment transport sub-model of AQUATOX has been successfully tested and is considered to be operational by the model developers.

Model Support, Usage and Usability

(1) Lacking a universal description of what a User's Manual should contain, all the models were found to provide adequate documentation. Typical documents introduce the principles and concepts of each model, describe the foundations of the algorithms, and describe the input required to run the models. However, there is a clear need for improvements in documentation to include a step-by-step tutorial of model use in order for a user to exploit all of a model's capabilities.

(2) The models under consideration generally lacked in GUI's and GIS linkage, with the exception of WASP6 and HSPF-RCHRES. Most model developers recognize the advantages realized by implementing user interfaces, and propose to include GUI's and GIS linkage in upcoming versions. However, *ease* in applying complex models is a mixed blessing. While experienced model users are empowered to make faster and more powerful applications, inexperienced users can fall into the trap of successfully running a model without fully understanding either (1) the background actions that the interface is performing in response to their instructions or (2) the underlying science that the model embodies.

(3) The degree and timeliness of human support available appears to vary widely. Realistically, the most comprehensive and consistent support appears to be available for a fee. Internet Listservers such as those provided for WASP and HSPF provide an effective means for modelers to help each other overcome obstacles encountered in their modeling efforts.

(4) Judging the application histories of the various models is complicated by the fact that most the models are evolving, and it is difficult to match application history to the specific scientific capabilities that were embodied in the version used for individual applications.

(5) The tools available for each model to perform data manipulation with the intent of providing the necessary input to each model (pre-processing) are not clearly documented or are outright lacking. While some models rely on third-party software (and its documentation) for pre-processing of data, description of the interface between the third-party tool and the model is generally not available.

(6) The tools available to perform post-processing of output data are also not clearly documented or outright lacking. Whether they are integrated with the GUI and GIS capabilities also seems to be unclear or missing completely in most model documentation

<u>Model Linkage Issues and Strategies</u>

(1) A generic information exchange mechanism was proposed that would mediate the coupling between any two models within a watershed-waterbody modeling system (WWMS). This approach simplifies the investigation, and later implementation, of coupling between all possible pairs of models.

(2) Criteria for evaluating the linkage compatibility of models were identified. Two operational criteria (input/output encapsulation and code encapsulation) and three conceptual criteria (time resolution, space resolution, scientific compatibility) were identified as critical to linkage potential.

(3) The next step in further development of a watershed-waterbody linkage would be a detailed specification of the proposed generic information exchange structure. Such a specification will hypothesize a "dataset" as a fundamental unit of information. A comprehensive and hierarchical listing of required datasets, methods of query and storage of datasets, as well as methods of transformation of one dataset to another would form the high level specification. The low-level specification will be the implementation of these "dataset" structures and methods in a programming language. The evaluation criteria for each model would measure how comprehensively the model provides the components required in the WWMS and how much programming effort is required to provide these components. Compatibility of any candidate pair of models could be assessed by how well the inputs of one match the datasets made available

by the outputs of the other.

WWMS is proposed as an inclusive, not an exclusive approach. An integration approach that excludes some models and includes only a few of available useful models implies the use of a ranking method. No ranking method can be so universal so as to apply to all combinations of problem definitions and available resources encountered in environmental studies being done in the world. A named waterbody model likely exists because it was previously found useful in some applications. Thus a WWMS should facilitate, and not prevent, integration of all existing waterbody models with the watershed model most compatible to their specific input needs.

(4) If a model does not score very high on operational compatibility, it can be included in the system by use of wrappers/filters. Such middleware can be constructed by the developer or experienced users, effectively distributing the programming and maintenance effort without losing conformity to each other. For modular and generalized models like HSPF, it may be more appropriate to skip the middleware step, and recode them to exchange information natively to/from the WWMS.

(5) If a model does not score very high on conceptual compatibility with a large number of other models, its presence in the WWMS suite would not impose any programming or run-time overhead on models that do not use inputs from it. In this sense, the WWMS is intended as an all-inclusive approach. Models that do not fit very well with other models because of non-standard process formulations or non-standard file input and output, nevertheless may be the most appropriate models for some problem definitions.

# 1.0 INTRODUCTION

This report constitutes the Final Report of a work assignment entitled "Evaluation of Contaminated Sediment Fate and Transport Models." The report summarizes the results included in two previous reports for Task 1 (Stoddard et al., 2002a) and Task 2 (Stoddard et al., 2002b), and expands upon them to describe the results of the final two study tasks (Tasks 3 and 4). Task 3 entailed conducting a comprehensive evaluation and comparison of the models that satisfied a preliminary screening (Study Task 2). These models constitute those that are judged the most promising for use in a broad range of waterbody types. Task 4 entailed an evaluation of the models for possible linkage with comprehensive watershed models such as the Hydrological Simulation Program - FORTRAN (HSPF) (Bicknell et al., 2001). The purpose of this evaluation was to ascertain the relative "compatibility" of each model with a model such as HSPF, and to identify potential problems in implementing a linkage. Compatibility issues that were considered include mismatches in model paradigms; irresolvable mismatches between HSPF watershed model outputs and required receiving water model inputs; and other conceptual issues.

## 1.1 Background

EPA's Office of Research and Development (ORD) is 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. ORD has proposed projects for funding by OERR that include a broad range of model evaluation, development and application activities and products. Identified research needs include a proof of concept for modeling alternative futures for a Superfund site; development of new modules for selected fate and transport models for certain types of water bodies; evaluation of the accuracy of the upgraded models by long-term modeling of a demonstration site; and providing a consensus framework for modeling remedial alternatives in large waterbodies.

To this end, EPA ORD's National Exposure Research Laboratory is providing support through its Ecosystem Research Division (ERD) in Athens, Georgia. To begin the support effort, an initial project has been formulated and undertaken to perform an evaluation of currently available numerical models usable for assessing fate and transport of contaminated sediments.
Recently OERR funded a similar study, completed by Tetra Tech (2000). The Tetra Tech study provides a comprehensive and essentially current evaluation of contaminated sediment model components. The objective of the study was to identify the best available models for supporting site-specific contaminated sediment remedial action decisions. A set of minimum requirements was established for each of three primary components (hydrodynamic, sediment transport, contaminant transport and fate) and three supplementary components (ecosystem, mixing zone, hydrologic). Models of each component type were screened, and those satisfying minimum requirements were identified. The minimum requirements established and applied in the study resulted in a varying number of survivors for each modeling component: 13 hydrodynamic models, 12 sediment transport models, 9 contaminant transport and fate models, 11 ecosystem models, 4 near-field models, and 5 hydrologic models. The model components that survived the screening process were further evaluated in terms of their applicability to various water body types (near field, 1-D, 2-D(*h*), 2-D (*v*), 3-D), their linkage capabilities, and their capability to represent site-specific processes. Seven linked modeling systems were identified that include the three primary components and satisfy all needs for modeling site-specific contaminated sediment conditions.

ERD Athens has a respected history of environmental model development, and has considerable expertise across the full range of modeling components required for comprehensive analysis of contaminated sediment problems. To successfully support OERR's research needs for expanded modeling capabilities, ERD desires to identify a small number of models that are judged superior to all others in their promise as tools for contaminated sediment analysis. Given practical considerations, a model's superiority is determined not only by its scientific and operational features, but by issues such as model availability, model support, and application experience. When the most promising models have been identified, ERD needs a basis on which to objectively compare these models and select one or more as the "chassis" into which model enhancements may be built. Such a selection process requires a head-to-head comparison of these models using a level of detail not currently documented.

A particular strength that ERD holds is in model development and modeling of the external loadings of contaminants from the land surface and subsurface. ERD has been a long-time focal point for development and support of the Hydrologic Simulation Program- FORTRAN (HSPF), perhaps the most versatile watershed model available in the public domain. Hence linkage of HSPF, or a watershed model of comparable complexity, into a more comprehensive contaminated modeling system is a topic of interest for both ERD and OERR.

## 1.2 Study and Report Objectives

### 1.2.1 Study Objectives

This review is the first task in a multi-year project. The ultimate goal is to upgrade the toxic transport and fate capabilities of the models ranked best for a variety of surface water body classes (e.g., low order stream, rivers, reservoirs, lakes, estuaries, coastal seas). The review will be followed up by testing the most promising models using available environmental data sets. The planned final step will be to develop new modules (for the appropriate models) that represent specific toxic transport/transformation processes that are not currently represented in the available models.

For this work assignment an evaluation of currently available numerical models useful for assessing fate and transport of contaminated sediments was performed and documented. The results of the evaluation will be used to support numerous aspects of a broader research and development effort at ERD that is focused on improving and demonstrating contaminated sediment models and modeling capabilities. A first objective of the study is to identify a small number of models that are judged superior to all others in their promise as tools for contaminated sediment analysis over a broad range of water body environments. Having achieved this, a second objective is to provide ERD with a basis on which to objectively compare these models and select one or more as the "chassis" into which model enhancements may be built. Such a selection process requires a head-to-head comparison of these models using a level of detail not currently documented. The final objective of this study is to evaluate issues and strategies involved in linkage of the select contaminated sediment models to the Hydrological Simulation Program - FORTRAN (HSPF) (Bicknell et al., 2001), or a similar comprehensive watershed model.

### 1.2.2 Report Objectives

This report constitutes the Final Report of a work assignment entitled "Evaluation of Contaminated Sediment Fate and Transport Models." The report summarizes the results included in two previous reports for Tasks 1 and 2, and expands upon them to describe the results of the final two study tasks (Tasks 3 and 4). Task 3 entailed conducting a comprehensive evaluation and comparison of the models that satisfied a preliminary screening (Study Task 2). These models constitute those that are judged the most promising for use in a broad range of waterbody types. Task 4 entailed an evaluation of the models for possible linkage with comprehensive watershed models such as the Hydrological Simulation Program - FORTRAN (HSPF). The purpose of this evaluation was to ascertain the relative "compatibility" of each model with a model such as HSPF, and to identify potential problems in implementing a linkage. Compatibility issues that were considered include mismatches in model paradigms; irresolvable mismatches between HSPF watershed model outputs and required receiving water model inputs; and other conceptual issues.

## 1.3 Overview of Aquatic Transport and Fate Models

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, with quantitative evaluations and comparisons of the effectiveness of alternative plans. Model frameworks can be applied to support evaluations of issues related to toxic chemicals contamination such as:

- Understanding key “cause and effect” processes and interactions that have influenced historical distributions of toxicants in the waterbody, sediment bed, and biota on a decadal time scale.

- Evaluating the effectiveness of alternative remediation scenarios, including “natural recovery”, in reducing toxicant contamination in the water column, sediment bed, and key target biota on a decadal time scale.

- Determining how many years will be required for “recovery” to achieve reduced toxicant levels in the sediments, fish and other target biota necessary to minimize the risks to human health and the environment.

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, 2000a).

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.

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.

### 1.3.1 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).

### 1.3.2 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).

### 1.3.3 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, 1999b) 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, 1999a) 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).

The pathways and interactions of solids and contaminants are governed by complex processes, and in almost all instances require an analysis using either an intermediate or advanced level of detail. Consequently, this study focuses on intermediate and advanced models.

## 1.4 Scope and Limitations

### 1.4.1 Study Scope

ERD has implicitly defined a preliminary scope for the model evaluation study by establishing a list of attributes that each model must possess. These include:

- 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 this model evaluation study within the constraints described above. In considering ERD's needs, we have made additional refinements to the scope that better define the modeling components that were, and were not, evaluated, and the range of model complexity that was, and was not, evaluated.

In addition, ERD's Statement of Work requires that the model evaluation identify and evaluate contaminated sediment models appropriate for application to a broad range of water bodies. For the purposes of this study, the Study Team has established a framework of water body classes; this framework and a description of the characteristics that was used to distinguish between different water body classes are provided in Section 3.2.

To fully address contaminated sediment issues, four modeling components must be considered: hydrodynamic models, sediment transport models, toxic chemical transport and fate models, and conventional pollutant transport and fate models. General features of the four model components are briefly described below.

Hydrodynamic Models*.* Use of time-varying, free-surface hydrodynamic computations to predict the movement of water in waterbodies with complex geometries is fundamental to a successful contaminated sediment transport and fate model application since advection and dispersion are the primary mechanisms for the transport of water quality constituents in the water column. Hydrodynamic models have generally been developed to apply to specific classes of waterbodies where certain simplifying assumptions can be made. For that reason, the criteria presented here consider the different types of waterbodies as well as the assumptions, features, model formulations and numerical methods used in hydrodynamic models.

Sediment Transport Models. Sediment transport models calculate the physical transport of sediment to which contaminants may be sorbed. It simulates the movement of bed load and suspended sediment in the water column due to ambient currents, turbulent diffusion and gravitational settling, and the exchange of suspended sediment due to deposition and resuspension. Sediment transport models consider fluxes of one or more sediment types across the boundaries of one or more bed layers. They also account for the spatial and temporal variations in the deposited sediment mass and geo-mechanical properties of the bed such as bulk density and shear strength.

Toxic Chemical Transport and Fate Models. Chemical fate models represent a number of physical-chemical kinetic processes including the adsorption and desorption of a toxicant with solids and organic matter. Because of the interaction of toxic chemicals with organic matter and suspended sediments, chemical fate models are designed to explicitly account for the interaction of solids with partitioning of the toxicant in the water column and sediment bed. Toxic chemical models consider the fate and transport of one or more contaminants across the boundaries of one or more bed layers. The coupling of a well-developed hydrodynamic and sediment transport model with a toxic chemical transport and fate model for natural water systems is the key component of a modeling framework for toxic organic chemicals and heavy metals that can be used to evaluate risk management scenarios based on the effectiveness of alternative remediation strategies.

Conventional Pollutants and Eutrophication Models. This class of model is included in our comprehensive inventory and evaluation of contaminated sediment transport and chemical fate models for two reasons: (1) toxic contaminants have a preferential tendency to adsorb both to fine-grained inorganic solids (e.g., clays and silts) <u>and</u> to particulate organic matter; and (2) in much the same manner as inorganic sediment, particulate organic matter and associated adsorbed contaminants are exchanged between the water column and the sediment bed by settling, deposition and resuspension. Particulate organic matter in a waterbody is derived from (a) external loading from watershed runoff and point source discharges, and (b) internal biological processes. Water quality models of conventional pollutants simulate the pathways and cycling of water quality constituents such as carbon, nutrients, dissolved oxygen, bacteria and pH in the water column and at the interface of the water column and sediment bed. Since the 1970s, water quality models have been developed to incorporate biologically-mediated pathways of carbon, nutrients and dissolved oxygen based on eutrophication models of one or more species groups of algae as primary producers in the aquatic food web. Particulate organic matter is thus represented in eutrophication models as the carbon equivalent of living (algae) and non-living (detritus) particulate material. Water quality and eutrophication models should include accurate numerical advection and dispersion schemes and a range of kinetic processes to represent the pathways and transformations of carbon, nutrients, algae and dissolved oxygen and other relevant state variables. Conventional pollutant and eutrophication models consider the exchange fluxes of various forms of water quality constituents across the sediment–water interface of the surficial sediment bed and across the boundaries of one or more deep sediment bed layers.

Figure 1.1 illustrates the connectivity of the modeling components that determine contaminated sediment transport and fate.

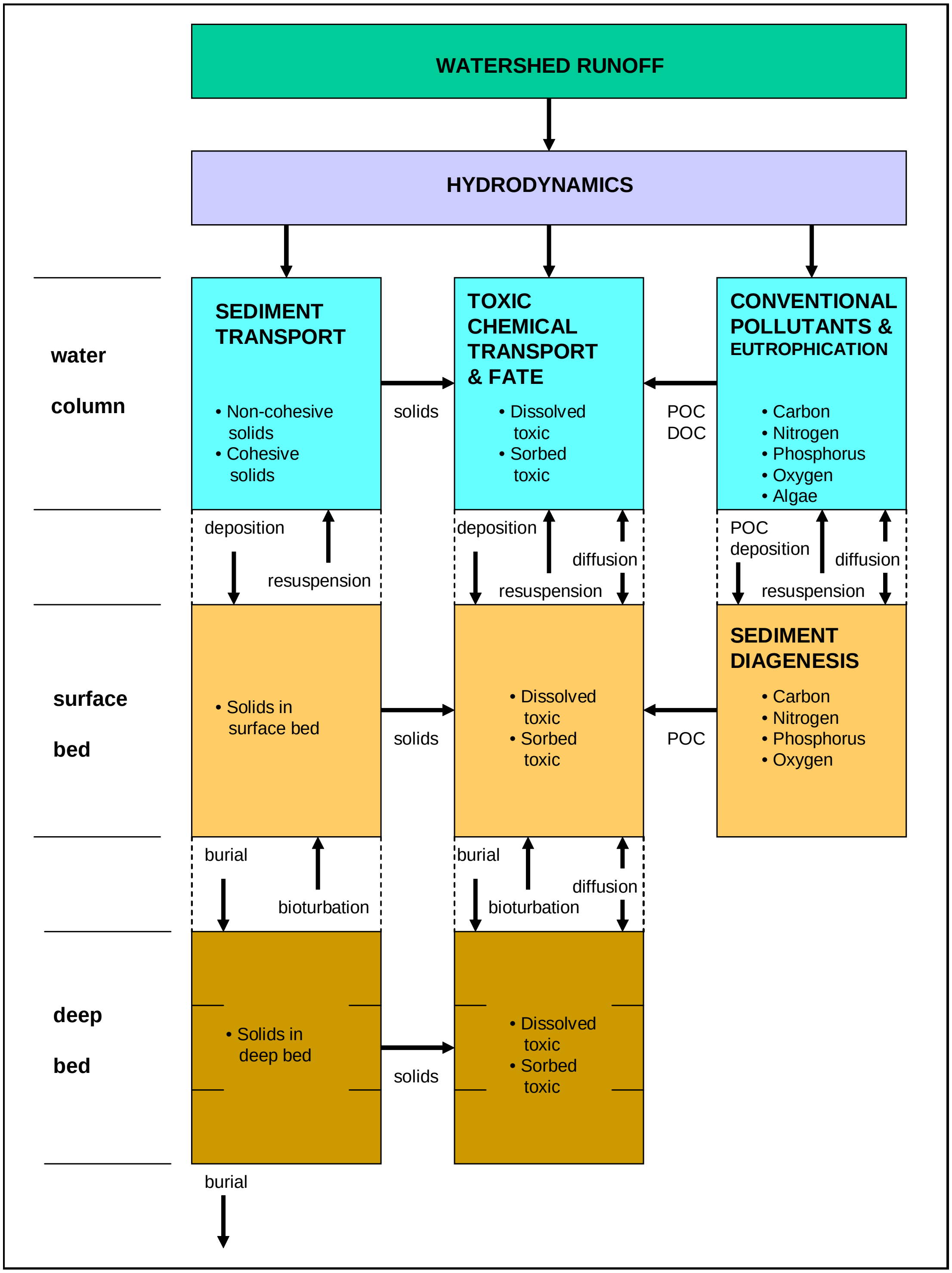


Figure 1.1. Contaminated sediment fate and transport modeling components.

This study <u>does not</u> evaluate near-field models, ecological models, or watershed loadings models. We have interpreted ERD's interest in investigating linkages between contaminated sediment models and watershed loadings models as an indication that single-source, near-field analysis is not the focal point of this study. The study background information provided by ERD indicated that the *immediate* focus of ERD's support to OERR is limited to sediment-related issues, and not bioaccumulation; hence, ecological models are not considered at this time. Finally, watershed loading models are only considered in the Task 4 analysis of linkage issues.

The pathways and interactions of solids and contaminants are governed by complex processes, and in almost all instances require an analysis using either an intermediate or advanced level of detail. 'First-tier' scientific criteria established minimum requirements for the scientific algorithms contained in candidate models; these criteria were used to screen models with the intent to eliminate models with an insufficient level of scientific detail (i.e., screening level models).

### 1.4.2 Study Limitations

It was not the intent of this study to provide full characterization of models with regard to the first-tier, or screening, criteria. For the sake of expedience, a "one strike and you're out" approach was utilized. During the screening process, as soon as a model failed one criterion, documentation of this failure was made, and the model was not further considered. It was also not the intent of this study to identify the "best" model for use in any one setting. Rather, the goal was to document, with considerable detail, a comparison between the most promising models of important modeling features and capabilities. It is anticipated that this documented comparison will provide a sound basis for selecting the models best suited for numerous research applications carried out at ERD and elsewhere.

## 1.5 Report Organization

Section 2 of the report describes the study methodology. In Section 2.1 the model screening criteria are identified for the four contaminated sediment modeling component groups. Section 2.2 describes the methods used to identify candidate models, and the two steps of screening that were used to select the model components that were moved forward in the study for detailed evaluation and comparison. Section 2.3 explains the methods that were used to perform the comprehensive evaluation of the selected models; methods used for evaluating both model science and model support and usage are described. In Section 2.4, the approach used to investigate linkage issues between the selected receiving water models and a comprehensive watershed model is described.

Section 3 of the report presents the results of the study. Section 3.1 provides the results of the initial and final screening of the candidate models. The section ends with a brief discussion of additional promising models that failed to meet one or more of the screening criteria. Section 3.2 presents the results of the model science evaluation for each of the four contaminated sediment modeling components, and Section 3.3 presents a parallel evaluation of model support and usability. Since model support and usability features are commonly shared among all components of a particular modeling system, the latter evaluation addresses modeling systems as a whole, rather than by component. Section 3.4 provides the results of our analysis of issues related to linking the models considered in this study to a comprehensive watershed model.

Section 4 presents the Study Team's conclusions and recommendations.

The report includes three appendices. Appendix A provides the results of the initial screening process. Appendix B provides physical descriptions of various waterbody types to which contaminated sediment models need to be applied. Appendix C describes the project QA/QC that was carried out throughout the study.

# 2.0 STUDY METHODOLOGY

In 1999 EPA ERD funded a similar, comprehensive evaluation of conventional pollutant/eutrophication models (HydroGeoLogic, 1999) that provides a starting place for developing the methodology needed for performing the current evaluation of contaminated sediment models. In the HydroGeoLogic study, an initial screening of available models resulted in identification of seven superior models that were subsequently evaluated and compared at a very detailed level. The science of the hydrodynamic, sediment transport and nutrient/plankton components of each of the seven models was evaluated independently. A similar approach was applied to this study.

The study methodology for the current study was comprised of the following elements:

- Developing screening criteria
- Identifying and screening candidate models
- Performing comprehensive model comparisons
- Evaluating model linkage issues
- Documenting models

## 2.1 Developing Screening Criteria

The objective of establishing and applying first-tier, or screening, criteria was to identify the contaminated sediment modeling components that offer ERD the most advantage as tools for carrying out a variety of model research and development activities. The screening criteria were applied to a comprehensive list of contaminated sediment modeling components. Model components satisfying *all* requirements were further evaluated and compared using more detailed second-tier, or comparison, criteria (Sections 3.2 and 3.3). A unique set of screening criteria were developed for application to each of the four modeling components (Section 1.3) that determine contaminated sediment transport and fate.

EPA established a list of evaluation criteria that must be considered in the model evaluation performed for the study. These include:

- 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.

We translated all the above considerations except the final one into explicit requirements and included them among the model screening criteria. The final criterion, consideration of models' amenability for linkage to a watershed model, requires considerable effort that builds on the detailed evaluation of each model's science and theory. Elements of this evaluation were performed in Tasks 3 and 4, and only on those models that satisfied the initial screening that was performed in Task 2. To complete the process of identifying detailed screening criteria for this study, we reviewed relevant criteria used in four recent model evaluations (WEST Consultants, 1996; HydroGeoLogic, 1999; Tetra Tech, 2000; Fitzpatrick et al., 2001). Taking into consideration the objectives and institutional context of the current model evaluation, we used these supplemental studies to identify additional screening criteria as deemed appropriate.

We established two types of screening criteria: scientific criteria and "general" criteria related to model support and usage. The general criteria identified below were applied to models in *all* model component groups.

### 2.1.1 General Criteria

EPA established three general criteria that are applicable to all components:

- 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, up-to-date documentation/user manual.
- Model must have an adequate history of application.

The Study Team refined all three of these criteria in order to make more objective determinations of whether candidate models were truly the most beneficial to ERD for its planned research and development activities. Given that ERD anticipates modifying/enhancing the code of the selected models, we determined that the most important issue related to availability of a proprietary model was that the source code of the model be available for modification. Regarding the minimum requirements for model support, we developed two discrete criteria, one for human support and one for documentation. We determined that human support must be available via telephone, Internet, or personal contact. The support need not be *gratis*, but it must be available. Regarding the nature of documentation, we expanded and refined the requirement to include either printed or model-embedded (i.e., interactive) documentation, and we provided a more explicit requirement for documentation content.

Regarding the requirement for a track record of credible model application, we determined that either (1) documented peer review by one or more technical experts or (2) publication of an application in a peer-reviewed journal reflects an "adequate history of application." In lieu of peer review, three documented applications were also deemed as adequate proof of credible and sufficient application.

With these refinements to the general first-tier model requirements, the resulting criteria are as follows:

*Criterion G1: Availability*. Model source code must be available to ERD for modification. If the model is proprietary, then the model, all source code and documentation must be available for purchase without run-time license requirements. All computer source code and all related files used to compile and execute the model must be available in electronic format.

*Criterion G2: Human Model Support.* Technical support must be readily available for the model; support may be provided via telephone, Internet correspondence, or personal contact, and need not be provided without fee.

*Criterion G3: Documentation.* Model documentation and user instructions must be available either in printed form or as an interactive resource embedded in the model package itself. User instructions on input and output operations for the current release must be available, as well as documentation of the model's governing equations, their transformation to solvable forms, and any supporting algorithms. Model documentation must also make clear the limitations and the environmental conditions under which the model can be appropriately applied.

*Criterion G4: Application History.* The model must have a proven track record of successful applications to real world problems. One of three criteria must be met. Either (1) an application of the model must have undergone peer review by an expert (or panel of experts) with the results of the review published in the open literature, or (2) an application of the model must have been published in a peer-reviewed journal, or (3) the model 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.

### 2.1.2 Sediment Transport Criteria

The screening criteria applied to sediment transport models in this study include all general criteria listed in Section 2.1.1, plus a set of additional criteria specific to the sediment transport model class.

*Criterion S1: Conservation of Mass.* The sediment transport model should be based on an appropriate solution of the time-variable mass continuity equation for suspended solids transported in the water column and solids exchanged between the water column and the sediment bed. A sediment transport model that provides only flow and velocity dependent estimates of the carrying capacity of a river for solids without consideration of the coupling of solids between the water column and sediment bed is not based on a complete mass balance of solids. This type of model would not satisfy first-tier criteria and thus would not be considered as a candidate for further consideration in the detailed analysis.

Mass conserving, accurate and stable numerical solution techniques are essential to describe the transport of solids in the water column and the coupling of solids between the water column and the sediment bed. The numerical solution scheme for the mass balance should be based on accepted formulations available in the literature.

*Criterion S2: Coupling of Water Column and Sediment Bed.* In order to explicitly represent deposition and resuspension of solids, the sediment transport model for a waterbody should provide a minimum vertical representation as follows: (a) single water column layer coupled with (b) surficial sediment bed. The explicit coupling of solids between the water column and sediment bed should be represented in the sediment transport model by allowing for either (a) externally provided or (b) internally simulated specification of: (i) settling/deposition velocity; (ii) resuspension velocity; and the (iii) distribution of solids concentration in the water column and the surficial sediment bed. In addition, the model should be able to define the time and space dependency of the deposition and resuspension velocities for each particle class.

*Criterion S3: Spatial Dependence of Initial Conditions.* The sediment transport model should be able to accept spatially varying initial conditions of solids concentrations, or mass, for the water column and the sediment bed. The model should be able to accept both user defined initial conditions (“cold starts”) as well as initial conditions defined by model results at the termination of a previous simulation run ("re-starts").

*Criterion S4: Point and Nonpoint Source Boundary Inputs.* The sediment transport model should allow for the specification of time-varying 'point source' boundary condition inputs to the waterbody at arbitrary multiple locations consistent with the boundary inflows defined by flow inputs to the hydrodynamic model. The sediment transport model should allow for explicit representation of external mass loads from 'point sources' such as that contributed by (a) tributaries; (b) municipal and industrial wastewater discharges; (c) urban stormwater runoff; and (d) combined sewer overflows. The model should also be able to account for the 'point source' load inputs of solids from open water disposal of dredged spoil material, sewage sludge or contaminated soils. The sediment transport model must also be able to accept continuous time series of external nonpoint source loading rates of solids for a range of typical low-flow, base flow and high flow conditions characteristic of the water body. Nonpoint source loading of solids is typically obtained from the results of a watershed model as direct runoff from sub-watersheds into a set of reaches of the physical domain defined for the hydrodynamic and sediment transport model.

*Criterion S5: Linkage to Toxic Chemical Fate Model.* The results of the sediment transport model must be able to be linked with a toxic chemical transport and fate model to interface the solids concentrations simulated in the water column and the sediment bed as input data for the partition calculations of the toxic contaminant fate model. Since solids in the water column and the sediment bed do not influence the toxic chemical concentration, the results of the sediment transport model can be provided to the toxic chemical fate model by either (a) internal coupling of a sediment transport model with a toxic fate model within a single model framework or (b) external linkage of the results of the sediment transport model as input to a toxic chemical model.

### 2.1.3 Toxic Chemical Transport and Fate Criteria

The screening criteria applied to toxic chemical transport and fate models in this study include all general criteria listed in Section 2.1.1, plus a set of additional criteria specific to the toxic chemical transport and fate model class.

*Criterion T1: Conservation of Mass.* The toxic chemical transport and fate model should be based on an appropriate solution of the time-variable mass continuity equation for a toxicant transported in the water column and exchanged between the water column and the sediment bed. A toxic chemical transport and fate model that only provides the distribution of toxicant in the water column without explicit consideration of the coupling of the toxicant between the water column and sediment bed is not based on a complete mass balance of a toxic chemical. This type of model would not satisfy first-tier criteria and thus would not be considered as a candidate for further consideration in the detailed analysis. Mass conserving, accurate and stable numerical solution techniques are essential to describe the transport of a toxicant in the water column and the coupling of the toxicant between the water column and the sediment bed. The numerical solution scheme for the mass balance should be based on accepted formulations available in the literature.

*Criterion T2: Coupling of Water Column and Sediment Bed.* In order to explicitly represent the interaction of a toxicant sorbed onto solids and the deposition and resuspension of solids, the toxic chemical transport and fate model should allow for at least a two-layer vertical representation of a waterbody as a water column layer coupled with a surficial sediment bed. The explicit coupling of a toxicant in the water column with the sediment bed should be represented in the model by allowing for the vertical exchange of the (a) dissolved fraction of a toxicant by diffusive mixing between the water column and pore water of the bed; (b) particulate fraction of a toxicant by deposition and resuspension of solids. In order to represent the vertical exchange of a toxicant, the distribution of the total toxicant concentration must be explicitly simulated in the water column and the surficial sediment bed and the model should be able to allow for the input of different partition coefficients assigned to the water column and the sediment bed.

*Criterion T3: Kinetic Processes and Interactions.* The toxicant model must allow for the explicit representation of the physical-chemical processes that determine the kinetic fate of the toxicant. The model must be able to explicitly allow for the following kinetic processes: partitioning of the toxicant with solids, volatilization, hydrolysis, photolysis, oxidation and biodegradation. A toxic chemical model that accounts only for an overall "lumped" loss of the toxicant from the water column as a composite of physical-chemical processes would not pass first-tier criteria since this type of model is so highly simplified that it is not technically acceptable for further consideration as a candidate model.

*Criterion T4: Spatial Dependence of Initial Conditions.* The toxic chemical transport and fate model should be able to accept spatially varying initial conditions of toxicant concentration, or mass, for both the water column and the surficial sediment bed. For sediment transport and chemical fate models that define multiple sediment bed layers, the model should be able to accept different toxicant concentrations assigned to each vertical layer of the sediment bed as spatially dependent initial conditions to represent a potential source of toxicant that can be present in subsurface deep bed layers as a result of historical practices for the disposal of toxic materials to a waterbody. The model should be able to accept both user defined input of initial conditions ("cold starts") as well as initial conditions defined as data generated by model results at the termination of a previous simulation run ("re-starts").

*Criterion T5: Point and Nonpoint Source Boundary Inputs.* The toxic chemical transport and fate model should allow for the specification of time-varying 'point source' boundary condition inputs to the waterbody at arbitrary multiple locations consistent with the boundary inflows defined by flow inputs to the hydrodynamic model and the inputs of solids to the sediment transport model. The toxic chemical transport and fate model should allow for explicit representation of external mass loads of toxicant from 'point sources' such as that contributed by (a) tributaries; (b) municipal and industrial wastewater discharges; (c) urban stormwater runoff; and (d) combined sewer overflows. The model should also be able to account for the 'point source' load inputs of toxicant from open water disposal of dredged spoil material, sewage sludge or contaminated soils. The toxic chemical transport and fate model must also be able to accept continuous time series of external nonpoint source loading rates of toxicant for a range of typical low-flow, base flow and high flow conditions characteristic of the water body. Tributary inputs and nonpoint source loading of a toxicant is obtained either from (a) flow-dependent rating curves or (b) the results of a watershed model as direct runoff from sub-watersheds into a set of reaches of the physical domain defined for the hydrodynamic, sediment transport and toxic chemical models.

*Criterion T6: Linkage with Sediment Transport Model.* The results of a sediment transport model must be able to be linked as input to a toxic chemical transport and fate model to interface the solids concentrations simulated in the water column and the sediment bed as input data for the partition calculations of the toxic contaminant fate model. Since solids in the water column and the sediment bed do not influence the toxic chemical concentration, the results of the sediment transport model can be interfaced with a toxic chemical fate model by either (a) internal coupling of the sediment transport model with the toxic fate model within a single model framework or (b) external linkage of the results of the sediment transport model as input to a toxic chemical model.

### 2.1.4 Conventional Pollutant Transport and Fate Criteria

The screening criteria applied to conventional pollutant and eutrophication models in this study include all general criteria listed in Section 2.1.1, plus a set of additional criteria specific to the conventional pollutant eutrophication model class.

*Criterion C1: Conservation of Mass.* The conventional pollutant transport and fate model should be based on an appropriate solution of the time-variable mass continuity equation for a pollutant transported in the water column and exchanged between the water column and the sediment bed. A conventional pollutant transport and fate model that only provides the distribution of pollutant in the water column without explicit consideration of the coupling of the pollutant between the water column and sediment bed is not based on a complete mass balance. This type of model would not satisfy first-tier criteria and thus would not be considered as a candidate for further consideration in the detailed analysis. Mass conserving, accurate and stable numerical solution techniques are essential to describe the transport of a conventional pollutant in the water column and the coupling of the pollutant between the water column and the sediment bed. The numerical solution scheme for the mass balance should be based on accepted formulations available in the literature.

*Criterion C2: Coupling of Water Column and Sediment Bed.* In conventional water quality and eutrophication models, particulate materials settle onto the sediment bed and can be resuspended from the sediment bed back into the water column. Dissolved constituents are transported between the surficial sediment bed and the water column by diffusive exchange of constituents between porewater and the water column at the sediment-water interface. In order to explicitly represent the interaction of a conventional pollutant sorbed onto solids (e.g., orthophosphate) and the deposition and resuspension of solids, the conventional pollutant transport and fate model should allow for at least a two-layer vertical representation of a waterbody as a water column layer coupled with a surficial sediment bed. The explicit coupling of a pollutant between the water column and the sediment bed should be represented in the model by allowing for the vertical exchange of the (a) dissolved fraction of a pollutant by diffusive mixing between the water column and pore water of the surficial bed; and the (b) particulate fraction of a pollutant by deposition and resuspension of solids. Vertical transport of the dissolved and particulate forms of a pollutant can be represented as either (a) externally provided input data to the model or (b) internally coupled data simulated by the model. A model that represents the vertical exchange of dissolved constituents, such as oxygen and nutrients, as externally provided benthic source or sink terms is acceptable even if a sediment bed is not explicitly included in the model domain. A model representing vertical transport of particulate matter as externally provided data to describe (a) deposition, (b) resuspension or (c) the net result of deposition and resuspension is acceptable. In order to represent the vertical exchange of a pollutant using internally simulated processes for deposition and resuspension of particulate matter and sediment diagenesis, the distribution of the total pollutant concentration must be explicitly simulated in the water column and the surficial sediment bed. The model should be able to allow for the input of different reaction coefficients assigned to the water column and the sediment bed. (Note: the wording of this criterion was refined by the Study Team subsequent to the Task 1 report to eliminate the impression that independent representation of the settling and resuspension processes is a prerequisite for satisfying this criterion.)

_Criterion C3: Kinetic Processes and Interactions._ The conventional pollutant model must allow for the explicit representation of the physical and biogeochemical processes that determine the pathways, kinetic fate and transformations of the pollutants. The model must be able to explicitly allow for the kinetic processes that affect carbon, nitrogen, phosphorus, oxygen and algal biomass.

_Criterion C4: Spatial Dependence of Initial Conditions._ The conventional pollutant transport and fate model should be able to accept spatially varying initial conditions of pollutant concentration, or mass, for both the water column and the surficial sediment bed. The model should be able to accept both user defined input of initial conditions ("cold starts") as well as initial conditions defined as data generated by model results at the termination of a previous simulation run ("re-starts").

_Criterion C5: Point and Nonpoint Source Boundary Inputs._ The conventional pollutant transport and fate model should allow for the specification of time-varying 'point source' boundary condition inputs to the waterbody at arbitrary multiple locations consistent with the boundary inflows defined by flow inputs to the hydrodynamic model and the inputs of solids to the sediment transport model. The conventional pollutant transport and fate model should allow for explicit representation of external mass loads of toxicant from 'point sources' such as that contributed by (a) tributaries; (b) municipal and industrial wastewater discharges; (c) urban stormwater runoff; and (d) combined sewer overflows. The model should also be able to account for the 'point source' load inputs of pollutant from open water disposal of dredged spoil material or sewage sludge. The conventional transport and fate model must also be able to accept continuous time series of external nonpoint source loading rates of pollutant for a range of typical low-flow, base flow and high flow conditions characteristic of the water body. Tributary inputs and nonpoint source loading of a pollutant is obtained either from (a) flow-dependent rating curves or (b) the results of a watershed model as direct runoff from sub-watersheds into a set of reaches of the physical domain defined for the hydrodynamic, sediment transport and toxic chemical models.

_Criterion C6: Linkage of Suspended Solids to Eutrophication Models._ The results of a sediment transport model, or at a minimum, the specification of site-specific suspended solids data, should be able to be linked to a conventional pollutant and eutrophication model to account for the influence of non-living suspended solids on light extinction and algal growth. The impact of suspended solids on light extinction can be represented within a conventional pollutant eutrophication model by either (a) internal coupling of the sediment transport model with the eutrophication model within a single model framework or (b) external linkage of the results of the sediment transport model as input to an eutrophication model; or (c) empirical specification of site-specific data to characterize time and space dependency of light extinction on suspended solids. (Note: the wording of this criterion was refined by the Study Team subsequent to the Task 1 report to eliminate the impression that computation and use of suspended solids output from a sediment transport model is a prerequisite for satisfying this criterion.)

*Criterion C7: Linkage of Suspended Solids and Organic Carbon to Contaminant Fate Models.* The results of the sediment transport model should be able to be linked as input to a toxicant fate model to provide input data for the suspended solids-based toxicant partitioning calculations. The results of the conventional pollutant and eutrophication model, or at a minimum, the specification of site-specific data, should be able to be linked as input to a toxicant fate model to provide dissolved organic carbon and particulate organic carbon data for the organic carbon-based toxicant partitioning calculations. Suspended solids data can be interfaced with a toxicant fate model by either (a) internal coupling of the sediment transport model to the toxicant model within a single model framework or (b) external linkage of the results of the sediment transport model as input to a toxicant fate model. Organic carbon data can be interfaced with a toxicant fate model by either (a) internal coupling of the eutrophication model to the toxicant model within a single model framework; (b) external linkage of the results of the eutrophication models as input to a toxicant fate model; or (c) empirical specification of site-specific data to characterize time and space dependency of organic carbon.

### 2.1.5 Hydrodynamics Criteria

The screening criteria applied to hydrodynamic models in this study include all general criteria listed in Section 2.1.1, plus a set of additional criteria specific to the hydrodynamic model class. All screening criteria used by Tetra Tech (2000) are included.

*Criterion H1: Linkage to Sediment Transport and Toxic Chemical Fate Models.* Either (1) the hydrodynamic model is internalized in one or more of the sediment transport and/or toxic chemical transport and fate models that have passed the first-tier screening, or (2) the hydrodynamic model has been successfully linked to one or more of these models. External linking information should include time varying water surface elevation or depth, bed elevation, mass conserving flows across cell continuity control volume boundaries, and bed stresses in continuity control volumes adjacent to the sediment bed.

*Criterion H2: Model Formulation.* The model should solve appropriate forms of the unsteady momentum, continuity and auxiliary mass transport equations in 1, 2 or 3 dimensions. The numerical solution scheme should be based on accepted and robust formulations. Accuracy, stability and conservation properties (momentum and mass) should be theoretically demonstrated and capable of being experimentally tested.

Criterion H3: Initial Conditions. The model should be capable of cold starts (arbitrary initial condition) or restarting for conditions at the end of a previous simulation.

*Criterion H4: Boundary Conditions and External Forcing Functions.* The model should include provisions for time varying boundary conditions including appropriate water surface elevation and/or flow conditions at open boundaries and volumetric source/sinks inside and along the waterbody domain boundary.

## 2.2 Identifying and Screening Candidate Models

### 2.2.1 Identifying Models

In order to identify a comprehensive list of currently existing contaminated sediment modeling components, we identified as many models as possible that include one or more of the following components: sediment transport, toxic chemical transport and fate, conventional pollutant transport and fate. Within the context of this study our interest in hydrodynamic models was restricted to identifying the best models that are commonly used to drive the transport computations contained in the "best" sediment and chemical models. Consequently, our goal was to identify selected hydrodynamic models subsequent to the identification of the sediment and chemical models.

Our approach to identifying candidate models was to first focus our attention on recent reviews and compendia of models, so as to gain immediate recognition of the most credible and commonly used models. Five very good references (Tetra Tech, 2000; HydroGeoLogic, 1999; Fitzpatrick et al., 2001; WEST Consultants, 1996, Limno-Tech, Inc., 2002) were identified to support this effort. These resources, all of which represent recent (1995 or later) efforts to identify the best of the currently available modeling tools, and all of which were prepared by professionals actively involved in water quality modeling, provided a strong starting point for identifying candidate models.

Other candidate models were identified using the WERF Model Selection Tool (Fitzpatrick et al., 2001). This tool provides an extensive list of sediment transport, hydrodynamic, chemical fate and transport, and water quality models, along with summary information describing each model. To ensure that our search for the most promising models was comprehensive, additional models were also investigated by means of phone calls to knowledgeable professionals, and by investigating a set of well-organized and comprehensive internet links provided on the USGS Surface-water quality and flow Modeling Interest Group (SMIG) web page. In addition, each of the participating firms used additional reference materials within their firms' libraries to supplement the search.

The complete lists of candidate models identified in the four model classes can be seen in Appendix A.

### 2.2.2 Preliminary Screening

Models were screened based upon the general screening categories (Section 2.1.1) and the screening categories specific to each model class (Sections 2.1.2 through 2.1.5). A screening grid was developed for each model class, containing a row representing each candidate model and a column representing each screening criterion.

Each member of the Study Team filled in the screening grids. For each candidate model, each team member indicated whether that model failed any one of the criteria. If the model failed one of the criteria, the team member did not continue to evaluate the model on the basis of the other criteria. If the team member found the model to pass all of the criteria, that information was noted as well. Once each team member filled the screening grids, the results were compiled into one master set of screening grids.

In many cases the members of the Study Team were familiar with a set of models and could fill in the grid without additional research. A small number of the models required additional research. In some cases team members responded with conflicting evaluations of the same model, and in these cases the conflicting evaluators were asked to discuss the reasons for their decisions. Through this process consensus was developed for each model. Once the master screening grids were developed, they were sent back to each team member for final review.

Since our study's intent was to perform detailed comparison of hydrodynamic models that are already used to drive the 'best' fate and transport models, the screening of hydrodynamic models necessitated an extra step. First, we compiled a list of hydrodynamic models known to be associated with sediment/chemical fate and transport models and applied the hydrodynamic model screening criteria. After the models that passed all screening criteria were identified, the list was further culled to eliminate models that did not have established linkages with models that passed the screening criteria of at least one of the other three contaminated sediment modeling components. For example, RIVMOD passed the hydrodynamic component screening, but did not pass any of the other three screenings (sediment, toxics, conventional pollutants), and hence was eliminated from further consideration.

It should be noted that the screening process was not devoid of subjectivity. As much as the Study Team tried to be objective, there were instances where familiarity with a certain model may have led to a model passing a criterion where someone not so familiar with the same model might have failed the model on the same criterion. The 'availability' criterion can be used as an example of this situation. Published documentation for one model might indicate that a model is proprietary and that its source code is not available. However, through familiarity with that model's developers a team member might have been aware that the developers would make an exception or change the distribution policy in response to the needs of this study and needs of subsequent elements of ERD's support program for OERR. That model would be judged to meet the 'availability' criterion, where without the personal contact the model would have been eliminated based on this criterion.

Another example of a case in which a subjective decision was made in the preliminary screening relates to models developed by HydroQual, Inc. HydroQual, which is clearly one of the premier environmental model developers, has made a corporate decision to make the source code for all their models available to the public for both modification and application. They began the process by releasing ECOMSED in early 2002; it was the goal of HydroQual to release to the public domain additional models with great strength in representing fate and transport of both toxic and conventional pollutants by the end of 2002. In making the decision to move these models forward through the preliminary screening, the Study Team anticipated that these models would meet the screening criteria by the time the study concluded.

It is possible that inaccurate evaluations could result from misinterpreted or misleading documentation. The Study Team assumed that documentation for each of the models is accurate; checking documentation against source code is beyond the scope of this study. As stated earlier, a 'one-strike-and-you're-out' policy was used in evaluating all models. This policy means that once a model failed one criterion the evaluation did not continue for other criteria, as that would have required a much greater effort without affecting the results of the screening process.

### 2.2.3 Final Screening

<u>Culling Models</u>

After the preliminary screening had been completed, the Study Team further scrutinized the remaining models, primarily by means of personal contact with the model developers. These correspondences uncovered a number of issues that had not been fully considered during the initial screening:

- Certain models that passed the initial screening are closely related, with older versions of the model included alongside newer versions that have enhanced capabilities.
- Certain models that passed the initial screening contain different capabilities for one modeling component group (e.g., hydrodynamics), but identical capabilities for one or more of the model component groups (e.g., sediment transport).
- Certain model versions that passed the initial screening evolved from models that clearly pass the screening criteria for application history and/or documentation, but the newer version is not yet supported by the required level of usage or documentation.
- Certain of the models, for one reason or another, do not fully satisfy the criterion related to model availability within the timeframe in which this study has been completed.

Armed with the additional information gained by discussions with the model developers, the Study Team and the WAM eliminated additional modeling components.

Joint Consideration of Models

A number of the model components that passed the final screening were fairly close 'cousins' to each other; i.e., the models are originally derived from the same parent model (e.g., WASP). The Study Team and the WAM agreed that the objectives of the study were best met by jointly addressing the capabilities of certain pairs of cousins by selecting one from among them for the detailed comparison. In these cases any significant differences between cousins have been identified as part of the description of the model chosen for detailed evaluation.

### 2.3 Performing Comprehensive Model Comparisons

The Study Team further evaluated the models that survived the screening effort by applying a more vigorous and comprehensive set of comparison criteria. As stated earlier, it was not the intent of this study to identify the "best" model for use in any one setting. Hence, the second-tier analysis was not a further screening. Rather, the goal was to document, with considerable detail, a comparison of important modeling features and capabilities for the most promising models in each class of the contaminated sediment modeling system. It is anticipated that this documented comparison will provide a sound basis for selecting the models best suited for numerous research applications carried out at ERD and elsewhere.

As was the case with the 'screening' criteria, 'comparison' criteria included both scientific considerations, and also model support and usability issues. The scientific comparison criteria are, of course, specific to each model class, whereas the model support and usability criteria (Section 3.3) are relevant to all models in all classes.

To provide clarity in documenting the results of model comparisons, comparison matrices were used. However, certain of the comparison criteria identified in this section do not lend themselves well to the 'yes-no' characterization used in matrices. For example, information characterizing the extent of model usage or model support cannot be adequately conveyed in a 'yes-no' format. In such cases text-based comparisons were used.

#### 2.3.1 Model Science

To perform the model science evaluation, the second-tier, or comparison criteria that had been established at the beginning of the study were translated and expanded into tables that compared the models included in each of the component groups on state variable-by-state variable and process-by-process levels. Generally speaking, the second-tier assessment of the science of selected models focused on (a) the capability of each model to represent key features, attributes, processes or interactions; and (b) the level of detail of the formulation(s) used to describe the processes or interactions.

### 2.3.2 Model Support

The true value of a model to potential modelers is determined at least as much by the availability of good model application support as it is by good science. Recognition of this fact is reflected in the minimum requirements for models that were established and described in Section 2.1. The minimum requirements consider availability of documentation, support offered by model developers/sponsors and documented model applications. Model support may be available in many forms including manuals and application reports, developer/sponsor assistance, user's groups, workshops, web sites, and recurring conferences/symposia.

In the second-tier evaluation, the preliminary assessment of model support was expanded to provide a comparison of the *level* of support associated with each model. The comparison of support available for the candidate models included consideration of the following criteria:

Documentation. We evaluated each model for the existence, availability and general quality of documentation, including the user's manual, discussion of theory, and coding structure.

Application aids. By examining the model user's manuals and interviewing the model developers/maintenance providers, we determined whether or not modeling techniques/tools (e.g., graphical user interfaces, pre- and post-processors, linkage capabilities to GIS) intended to enhance ease-of-use are available for each model.

Human support. We evaluated the availability of developer/sponsor assistance, user's groups, workshops, web sites, and recurring conferences/symposia.

Model usage. The model usage analysis had two components. First, we performed a general assessment of each model's application history. Second, we assessed the resource requirements (level of effort, data, user expertise) needed to apply each model.

When all the above criteria had been assessed, we used the results to develop a narrative comparison of the available support for the candidate models.

## 2.4 Evaluating Model Linkage Issues

Models were evaluated for possible linkage with comprehensive watershed models such as the Hydrological Simulation Program - FORTRAN (HSPF). The purpose of this evaluation was to ascertain the relative "compatibility" of each model with a model such as HSPF, and to identify potential problems in implementing a linkage. Compatibility issues that were considered include mismatches in model paradigms; irresolvable mismatches between HSPF watershed model outputs and required receiving water model inputs; and other conceptual issues.

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.

**2.5 Documenting Models**

Summary documentation was developed for each model for which detailed evaluation was performed. The documentation of model science is provided in the comparison tables included in Section 3.2, as well as the supporting text for the tables. The documentation of model support and usage is provided in Section 3.3. 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.

# 3.0 RESULTS

## 3.1 Screening of Models

A comprehensive collection of modeling systems and modeling system components were subjected to a two-phase screening process.  The details of the screening are provided below.

### 3.1.1 Initial Screening Results

One result of the screening was a determination that all but perhaps one of the conventional pollutant modeling components did not pass Criterion C7 (see Section 2.1.4).  Consequently, we eliminated this criterion, thereby relaxing our screening requirements to a level that an appropriate number of the best conventional pollutant models could be moved forward in the study for comparison.   The initial screening process identified the following models as most suitable for satisfying the needs of this study:

Hydrodynamic Models:
- CE-QUAL-W2 (Version 2)
- CH3D-WES (Version 1)
- ECOM-3D (Version 1.3 of ECOMSED)
- EFDC
- EFDC1D (Version 1)
- HSCTM-2D (Version 1)
- POM

Sediment Transport Models:
- AQUATOX (Version 3)
- CE-QUAL-ICM-TOXI (Version 1)
- ECOMSED (Version 1.3)
- EFDC
- EFDC1D (Version 1)
- HSCTM-2D (Version 1)
- HSPF-RCHRES (Version 12)
- IPX (Version 2.7.4)
- SEDZL
- WASP5(6)-TOXI5(6)

Toxic Chemical Fate and Transport Models:
- AQUATOX (Version 3)
- CE-QUAL-ICM-TOXI (Version 1)
- EFDC
- EFDC1D (Version 1)
- HSCTM-2D (Version 1)
- HSPF-RCHRES (Version 12)
- IPX (Version 2.7.4)
- RCA-TOX
- WASP5(6)-TOXI5(6)
- WASTOX

Conventional Pollutants and Eutrophication Models:
- AESOP
- AQUATOX (Version 3)
- CE-QUAL-ICM (Version 1)
- CE-QUAL-W2 (Version 2)
- EFDC
- EFDC1D (Version 1)
- HSPF-RCHRES (Version 12)
- RCA
- WASP5(6)-EUTRO5(6)

### 3.1.2 Final Screening Results

Culling Models

After the preliminary screening was complete, the Study Team further scrutinized the remaining models, primarily by means of personal contact with the model developers. These correspondences uncovered a number of issues that had not been fully considered during the initial screening:

- Certain models that passed the initial screening are closely related, with older versions of the model included alongside newer versions that have enhanced capabilities.
- Certain models that passed the initial screening contain different capabilities for one modeling component group (e.g., hydrodynamics), but identical capabilities for one or more of the model component groups (e.g., sediment transport).
- Certain model versions that passed the initial screening evolved from models that clearly pass the screening criteria for application history and/or documentation, but the newer version is not yet supported by the required level of usage or documentation.
- Certain of the models, for one reason or another, do not fully satisfy the criterion related to model availability within the timeframe in which this study has been completed.

Armed with the additional information gained by discussions with the model developers, the Study Team and the WAM eliminated additional modeling components using the rationale presented below.

**AESOP** was eliminated from the conventional pollutant fate and transport modeling component group. AESOP is the predecessor model of the WASP-EUTRO model, and does not contain significant positive features that have not been passed on to WASP-EUTRO.

**AQUATOX** (Version 3.0) was eliminated from the sediment transport modeling component group. This version of AQUATOX passed through the initial screening based on the fact that it includes the HSPF-RCHRES algorithms for internal computation of deposition and resuspension for three classes of inorganic solids combined with the capability to simulate multiple segments. However, the model developer suggested to us that, for studies requiring detailed sediment modeling, the intent has always been to use external hydrodynamic model and sediment transport models linked to AQUATOX's chemical and bioaccumulation modeling capabilities.

AQUATOX was preserved in the toxic chemical fate and transport and the conventional pollutant fate and transport modeling component groups.  However, it was necessary to revert back from version 3.0 to EPA version 2.0 in order to fully satisfy the screening criteria related to application history and documentation.

**CE-QUAL-ICM-TOXI** was eliminated from the sediment transport and the toxic chemical fate and transport modeling component groups.  There is not presently a version of the model available for release.  Changes to the code are presently underway, but at this time a timeline has not been established for producing an official release.

**CE-QUAL-W2** was eliminated from the conventional pollutant fate and transport and the hydrodynamic modeling components.  The final screening process was mindful of the fact that this study has its focus on two of the four modeling components: (1) sediment transport and (2) toxic chemical fate and transport.  As a result the Study Team had previously restricted the hydrodynamic models that were compared to only those that are known to be associated with sediment/chemical fate and transport models. Given the secondary nature of conventional modeling component, it was decided that a model would not be included in this group that did not contain a sediment or toxic chemical transport and fate module.

**RCA** was eliminated from the conventional pollutant fate and transport component group.  The model has traditionally been a proprietary product of HydroQual, but it is transitioning into the public domain.  The process of making the model's source code and documentation available is in progress, but the timing for completion of this study precludes the model from being included and adequately characterized.

**RCA-TOX** was eliminated from the toxic chemical fate and transport component group.  The model has traditionally been a proprietary product of HydroQual, but it is transitioning into the public domain.  The process of making the model's source code and documentation available is in progress, but the timing for completion of this study precludes the model from being included and adequately characterized.

**WASTOX** was eliminated from the toxic chemical fate and transport modeling component group. WASTOX is the predecessor model of the WASP-TOXI model, and does not contain significant positive features that have not been passed on to WASP-TOXI.

Joint Consideration of Models

A number of the model components that passed the initial screening are fairly close 'cousins' to each other; i.e., the models are originally derived from the same parent model (e.g., WASP). The Study Team and the WAM agreed that the objectives of the study were best met by jointly addressing the capabilities of certain pairs of cousins by selecting one from among them for the detailed comparison.  In these cases any significant differences between cousins have been identified as part of the description of the model chosen for detailed evaluation.  Model pairs, or cousins, include the following:

- ECOM-3D & POM (Hydrodynamic component)
- ECOMSED & SEDZL (Sediment component)
- EFDC & EFDC1D (Sediment, toxic chemical, and conventional pollutant components)

Final List of Models for Evaluation

The following models were identified as most suitable to be evaluated according to the detailed comparison criteria in the comprehensive model evaluation:

Hydrodynamic Models:
- CH3D-WES (Version 1)
- ECOM-3D/POM (ECOMSED Version 1.3)
- EFDC
- EFDC1D (Version 1)
- HSCTM-2D (Version 1)

Sediment Transport Models:
- ECOMSED & SEDZL (ECOMSED Version 1.3)
- EFDC & EFDC1D
- HSCTM-2D (Version 1)
- HSPF-RCHRES (Version 12)
- IPX (Version 2.7.4)
- WASP5(6)-TOXI5(6)

Toxic Chemical Fate and Transport Models:
- AQUATOX (Version 1.1)
- EFDC & EFDC1D
- HSCTM-2D (Version 1)
- HSPF-RCHRES (Version 12)
- IPX (Version 2.7.4)
- WASP5(6)-TOXI5(6)

Conventional Pollutants and Eutrophication Models:
- AQUATOX (Version 1.1)
- CE-QUAL-ICM (Version 1)
- EFDC & EFDC1D
- HSPF-RCHRES (Version 12)
- WASP5(6)-EUTRO5(6)

### 3.1.3 Other Promising Models

It should be noted that it has not been possible to include some of the premier models for evaluating contaminated sediment in our detailed evaluation. These models have been excluded from our study due to failure to meet the requirements for *immediate* availability to ERD and/or the lack of a sufficiently extensive and well documented application history. Noteworthy models that have been excluded from detailed evaluation are documented in a summary form below. Models that are included in this discussion are:

- CE-QUAL-ICM-TOXI
- QEA-FATE

- RCA
- RCA-TOX
- RTI version of WASP5-EUTRO5

CE-QUAL-ICM-TOXI

The CE-QUAL-ICM-TOXI model is an extension of CE-QUAL-ICM to allow its application to trace contaminants. The basic transport scheme and solution technique are common to both the eutrophication and trace chemical sub-models. The primary difference in the two models is in the number of state variables simulated (22 in the eutrophication model versus 8 in the trace chemical model), and in the form of the kinetic sources and sinks incorporated, since the processes controlling trace chemicals differ from those simulated in the eutrophication model. ICM/TOXI is designed to provide a broad framework applicable to many environmental problems and to allow the user to match the model complexity with the requirements of the problem.

ICM/TOXI simulates temperature, salinity, three solids classes and three types of chemicals. The three chemicals may be independent or they may be linked with reaction yields, such as a parent compound-daughter product sequence. Salinity and temperature are simulated in the same fashion as done with the eutrophication model. Salinity is treated as a conservative material. Temperature is simulated using the equilibrium temperature approach to describe surface heat exchange. Three solids types are included as well as a sediment bed model to allow prediction of the transport of sorbed contaminants and the impact of sorption on other kinetic processes.

Transformation and degradation processes simulated by ICM/TOXI include ionization, sorption, volatilization, biodegradation, photolysis, hydrolysis, and oxidation. Each chemical may exist as a neutral compound and up to four ionic species. The neutral and ionic species can exist in five phases: dissolved, sorbed to dissolved organic carbon (DOC), and sorbed to each of the up to three types of solids. Local equilibrium is assumed so that the distribution of the chemical between each of the species and phases is defined by distribution or partition coefficients. In this fashion, the concentration of any species in any phase can be calculated from the total chemical concentration. Therefore, only a single state variable representing total concentration is required for each chemical.

QEA-FATE

QEA-FATE is two-dimensional, vertically-averaged model that is capable of simulating hydrodynamics, sediment transport, and contaminant fate and transport in rivers, lakes and non-stratified coastal waters. The model is time-dependent and uses a non-orthogonal, curvilinear grid to represent complex geometry. The three sub-models (i.e., hydrodynamic, sediment transport and contaminant transport) are fully integrated and coupling of the sub-models is seamless. The sediment transport sub-model is an enhanced version of SEDZL, which is capable of simulating cohesive and non-cohesive suspended load transport, as well as bed load transport of coarse sand and gravel. A three-dimensional sediment bed model simulates temporal and spatial variations in bed properties, including bed armoring and consolidation effects. The contaminant fate and transport sub-model is used to predict changes in water column and sediment concentrations of particle-reactive chemicals. Fate and transport processes incorporated into the sub-model include: three-phase organic-carbon-based partitioning, volatilization, and first-order degradation kinetics. In addition, multiple chemicals can be modeled simultaneously, and kinetic routines to represent reactions between these state variables can easily be added to the framework. Chemical fate within the sediment bed is directly coupled with that in the water column, and is calculated using a Lagrangian numerical scheme that eliminates numerical dispersion. The processes of deposition, erosion, molecular diffusion, and particle mixing (i.e., bioturbation) are simulated within the sediment bed.

RCA

RCA is a generalized modeling framework capable of being used to address a wide-range of environmental water quality issues. RCA can trace its origins back to the WASP family of water quality modeling codes, developed for the USEPA by Hydroscience in the early 1970s. In a similar fashion to WASP, the user supplies a kinetic subroutine that describes the physical, chemical, and biological relationships between the relevant water quality constituents or state-variables of interest. While following a theoretical framework and code structure similar to the WASP computer codes, RCA differs from WASP in that the computational grids used by RCA are structured grids, while WASP uses a pointer schematization. The use of a structured grid system permits the RCA code to take advantage of computers capable of parallel processing, thus reducing program execution times.

The use of RCA requires the use of a companion hydrodynamic model ECOMSED (although RCA has been successfully linked to EFDC) in order to obtain advective and dispersive fields required to compute the movement of the water quality variables of interest within the study domain. To date kinetic subroutines have been developed for total and fecal coliforms, simple BOD/DO, eutrophication, calcium carbonate equilibrium chemistry, and emergent vegetation (sawgrass and cattails). The standard eutrophication kinetic subroutine considers two functional algal groups (winter diatoms and a summer mixed assemblage), various forms (particulate and dissolved, labile and refractory) of nutrients (C, N, P, Si), and dissolved oxygen and also includes an explicit sub-model of sediment diagenesis and nutrient fluxes. RCA makes use of a flexible input structure, which permits the user to assign pollutant inputs from point and diffuse sources, including atmospheric, as well as riverine and ocean boundaries, either as time-invariant or as time-variable inputs. RCA uses a simple first-order scheme for numerical integration (an Euler scheme), with an option for reducing the effects of numerical dispersion (Smolarkiewicz predictor-corrector).

RCA has been used in lacustrine, riverine, and estuarine studies, including Lake Erie, Onondaga Lake (NY), the Croton Reservoir (NY), Lake Victoria (East Africa) the upper Mississippi River, Jamaica Bay (NY), Green Bay (WI), Long Island Sound, the New York/New Jersey/New York Bight Complex, the Massachusetts Bays system, the Tar Pamlico Estuary, and Escambia Bay (FL).

RCA-TOX

RCA-TOX is derived from RCA and includes the concept of developing a site-specific kinetic subroutine for the chemical contaminants of interest. The kinetic subroutine defines the time rate of transfer of chemical between phases and transformation to degradation products. The standard RCA-TOX kinetic subroutine follows the theoretical framework utilized for US EPA's WASTOX and includes the processes of volatilization, photolysis, chemical hydrolysis, and microbial degradation.

For volatilization, the kinetic subroutine permits the user to select from different calculation procedures for determining the mass transfer coefficient depending on the waterbody type. The current version of RCA-TOX considers only direct photolysis, but does take into account light attenuation through the water column. In determining rates of hydrolysis for chemical contaminants, the RCA-TOX kinetics considers the effects of both temperature and pH, and, therefore, can consider acid, alkaline, and neutral hydrolysis. The user is required to input the rate constant for each hydrolysis type and the pH in each segment of the model.

While it is recognized that biodegradation encompasses a broad range of enzymatic processes by organisms on organic chemicals, the kinetics employed in RCA-TOX use a simplified approximation, which utilizes a first-order reaction rate and segment-specific bacterial biomass. For the adsorption of chemical contaminants to suspended matter, the RCA-TOX code uses a linear isotherm relationship to describe equilibrium sorption. The computer code does, however, consider multiple classes of suspended matter for chemical sorption, including phytoplankton carbon, detrital particulate organic carbon, and dissolved organic carbon.

While RCA-TOX does not explicitly model hydrodynamics, sediment transport, and organic carbon production, it can take these inputs from other models, such as ECOMSED and RCA, which are run off-line.

RCA-TOX has been applied to the Pawtuxet River (RI), a fate and transport model of mine tailings and copper in the Arafura Sea, Irian Jaya, Indonesia, and is currently being applied to a chemical fate and transport model for PCBs, PAHs, and Hg for the New York/New Jersey Harbor complex and the Passaic River, NJ.

Research Triangle Institute (RTI) Version of WASP5-EUTRO5

In addition to EPA's 'BASINS' modeling system, an alternative national-scale water quality model framework that integrates EPA's River Reach Files (RF1/RF3) and other EPA databases, has been developed by Research Triangle Institute (RTI) in Raleigh-Durham, NC. The National Water Pollution Control Assessment Model (NWPCAM) has been developed by RTI to evaluate the water quality and economic benefits that have been achieved by implementation of point source and nonpoint source water pollution control policies of the Clean Water Act. A modified version of WASP5-EUTRO5, developed by RTI, has been integrated in Version 2.0 of the National Water Pollution Control Assessment Model as the water quality model framework for nutrients, organic matter, dissolved oxygen and eutrophication (Bondelid et al., 2002). The RTI modifications to WASP5-EUTRO5 include inorganic suspended solids, salinity/chlorides, and fecal coliform bacteria as additional state variables for the eutrophication model. The formulation describing light extinction has been revised to include internally simulated algal biomass and the inorganic and organic components of suspended solids (Di Toro, 1978) to eliminate the need for an empirical 'parameterization' of non-algal light extinction. In the modified version of WASP5-EUTRO5, the modeler has the option of representing 'salt' as: salinity, chlorides, specific conductance or total dissolved solids. The mortality of coliform bacteria is dependent on water temperature, availability of light and the fraction of seawater using a formulation developed by Mancini (1978).

To facilitate the linkage of the modified WASP5-EUTRO5 model and WASP5-TOXI5 with EPA databases and the automated Reach File-based data processing scheme designed by RTI for implementation of the national-scale model, an innovative preprocessor program has been developed to automate the generation of the input files needed to execute WASP5-EUTRO5 and WASP5-TOXI5 for the river reaches of each of the 2,111 hydrologic catalog units in the 18 major river basins of the conterminous United States. The WASP5 pre-processor is designed to define the WASP5 segment grids as a laterally averaged water body or a branched network of tributaries in a watershed along the longitudinal (x) and vertical (z) dimensions. The preprocessor allows the flexibility to specify either a 1D(x) or 2D(x,z) spatial domain as: (a) single, or multiple, water column layers; and (b) zero, single or multiple sediment bed layers. A WASP5 post-processor program has also been developed to facilitate the extraction of the WASP5 simulation results to display model results as: (a) time series [C(t)]; (b) spatial transects [C(x)]; or (c) depth profiles [C(z)].

The modified version of WASP5-EUTRO5 has been applied as a component of the NWPCAM modeling system to streams, rivers, lakes and tidal waters in all 18 major river basins. The modified WASP5-EUTRO5 model has also been applied for "stand-alone" modeling studies of: Peconic Bay, NY; Norwalk Harbor, CT; the New River, WV; the Housatonic River, MA; and the Pirapama estuary in Brazil.

### 3.2 Model Science Evaluation

The central feature of contaminated sediment fate and transport models is the representation of solids in the water column and the bed. Figure 3.1 illustrates a holistic view of the breakdown components of solids in the aquatic environment without regard to a specific model framework. Each model of contaminated sediment fate and transport is built around a unique solids classification scheme that includes a sub-set of the classes that are represented in the figure; different models offer different schemes.

The model science evaluation in this study considers four components or compartments relevant to modeling contaminated sediment: hydrodynamics, sediment transport and fate, toxic chemical transport and fate, and conventional pollutant transport and fate. Since the objective of the study was to identify and evaluate the most promising models available for each of the four components independently, a different list of models is compared for each component. Some models are included in evaluations for more than one compartment.

<table>
<tr><th colspan="5">SOLIDS</th></tr>
<tr><td colspan="5">Organic and Inorganic</td></tr>
<tr><td colspan="2">Organic Matter</td><td colspan="3">Inorganic Matter</td></tr>
<tr><td>Living Biomass</td><td>Detritus</td><td>Silt</td><td>Clay</td><td>Sand</td></tr>
<tr><td colspan="5">Cohesive and Non-cohesive</td></tr>
<tr><td colspan="4">Cohesive</td><td>Non-Cohesive</td></tr>
<tr><td colspan="2">Organic Fines</td><td>Silt</td><td>Clay</td><td>Sand</td></tr>
</table>

Figure 3.1. Solids components in an aquatic environment.

Our approach to presenting the results of the model comparisons has been to use 'yes-no' answers within a series of comparison tables (Table 3.1 through 3.9). A red star in a particular row/column indicates that a given model *does* include the feature in question. In cases where a clarification is necessary, a footnote has been substituted for the star, and explanatory text has been included at the bottom of the table.

The tables examine and compare models using a high level of detail; the criteria embody a complex breadth of science. Attempting to define the terms and concepts embodied in the comparison criteria is beyond the scope of this report; the theory sections of user's manuals are the source of the scientific criteria that have been considered.

The criteria presented in the tables are intended to distinguish differences between models. Consequently, in most cases the tables indicate that certain models do not represent each feature, while others do. In cases where the tables indicate that none of the models include a particular feature, the feature has been included in the model comparison to indicate that it is considered a desirable feature. Such features are expanded upon in the discussion on recommended model enhancements (Section 4.0).

### 3.2.1 Sediment Transport Models

Sediment transport models are designed to represent the transport of suspended solids in the water column and the exchange of solids between the water column and the sediment bed. Suspended solids, the particles that remain in suspension in the water column, are transported in a waterbody by advection and turbulent mixing. Depending on the hydrodynamic characteristics of the waterbody, solid particles can be exchanged between the water column and the sediment bed by gravitational settling (deposition) and resuspension (bed erosion). Additional solids, predominantly coarse non-cohesive solids, can be transported as bed load in a thin layer near the bottom with the downstream transport of solids described by 'saltation', or rolling, sliding and hopping movement, of the individual particles.

As is typical for all categories of surface water models, sediment transport models have been developed over the past few decades as very simplified screening level models, intermediate level models applied for water quality management planning studies, and complex, or advanced, models developed for R&D studies and applied problem settings characterized by complex physical domains and a need for a high level of scientific credibility.

<u>Screening level</u> sediment transport models are typically designed to account only for the overall sedimentation loss of a single group of suspended solids from the water column. The loss rate of solids is parameterized as an effective settling velocity based on a long-term balance of deposition and resuspension. The solids available in the sediment bed are not represented in this type of a simple model. Screening level models are too simplified to be technically acceptable for the purposes of this study.

<u>Intermediate level</u> sediment transport models are designed to represent one or more classes of suspended solids in the water column and sediment bed, with the deposition and resuspension velocities of each size class of solids defined by external data and provided as input to the model. Intermediate level models represent the distribution of solids in both the water column and, at a minimum, the surficial sediment bed.

The most complex, or advanced, sediment transport models account for solids defined by (*a*) the suspended solids load of cohesive and non-cohesive materials transported and exchanged between the water column and sediment bed and (*b*) the bed load of non-cohesive solids transported near the sediment-water interface. Advanced sediment transport models internally compute deposition and resuspension velocities using functional formulations developed specifically for cohesive and non-cohesive classes of solids. Advanced sediment transport models explicitly represent the mass exchange of cohesive and non-cohesive solids deposited and eroded to and from the sediment bed to simulate the spatial and temporal changes in the elevation (i.e., thickness) of the surficial bed. Sediment bed consolidation processes can also be incorporated in advanced sediment transport models to account for the temporal changes in bulk density, porosity and shear stress of the bed as a geomechanical sediment bed model.

In reviewing and evaluating the various features or processes of a sediment transport model, the detailed assessment of candidate models focused on (*a)* the capability of a candidate model to represent a key feature, attribute, process or interaction; and (*b*) the level of detail of the formulation(s) used to describe the processes or interactions. When the model comparisons are used for selection of a model, the 'conceptual model' of the site-specific problem setting will determine which attributes of the head-to-head comparison are the most relevant. A Lamborghini or a Ferrari sports car may be the 'best' car available based on the criteria of achieving the fastest acceleration and ultimate speed. If, however, the specific use of the vehicle to be chosen is for off-road travel in a desert environment, selection of a high end sports car as the 'best' car available would be a very poor, and overly expensive choice. Similarly, the 'best' choice of a sediment transport model is entirely subject to the needs and criteria established by the 'conceptual model' for the problem setting of a specific project.

In comparing the attributes of candidate sediment transport models, the methods used in each model to represent the following model components were considered:

(1) Solids classes
(2) Deposition and resuspension of solids
(3) Cohesive solids
(4) Non-cohesive solids
(5) Bed load transport
(6) Surficial and deep sediment bed
(7) Coupling of hydrodynamic and sediment transport models: advection and dispersion
(8) Coupling of hydrodynamic and sediment transport models: bottom stress
(9) Coupling of hydrodynamic and sediment transport models: bathymetry
(10) Wetting and drying and particle trapping

A basis for comparing each of these ten components was established in the form of a 'comparison criterion.' The comparison criteria used for evaluating sediment transport and fate models in this study are as follows:

*Comparison S1: Representation of Solids Classes.* Sediment transport models are available with the following representations of single, and multiple, classes of solids: (*a*) single, "lumped" class of solids that is defined as neither cohesive or non-cohesive; (*b*) multiple classes of solids that are defined as neither cohesive or non-cohesive; (*c*) single, or multiple classes defined specifically as cohesive solids; (*d*) single, or multiple classes defined specifically as non-cohesive solids; (*e*) multiple classes defined specifically to represent both cohesive and non-cohesive solids. The 'conceptual model' of the site-specific problem setting must be used to provide insight into the number of size classes needed, and whether or not cohesive and/or non-cohesive solids must be considered as state variables for a site-specific project. Many rivers in the western states, for example, are dominated by non-cohesive solids in the water column and sediment bed. In contrast to western rivers, many estuarine water bodies are typically dominated by fine-grained cohesive particles. Models that represent only non-cohesive solids or only cohesive solids, rather than a more complex model that represents both cohesive and non-cohesive solids, would therefore be considered acceptable for these types of waterbodies.

Suspended solids measured in natural waters are comprised of both inorganic solids and particulate organic matter. Inorganic solids consist of cohesive fine-grained solids (clays and silts) and non-cohesive solids (sands, gravels, cobbles, boulders). Particulate organic matter consists of living biomass derived from primary producers (i.e., algae, macrophytes and benthic algae) and non-living detrital solids. Detritus is derived from external terrestrial sources via watershed runoff (e.g., leaf litter) and internal biological processes. The relative significance of how much particulate organic matter is represented as a component of suspended solids is defined by the ratio of particulate organic carbon to dry weight of solids as C/DW = POC/TSS. This ratio is also defined in the literature as the fraction of organic carbon (Foc). In a biologically productive (i.e., eutrophic) waterbody where the quantity of suspended solids can be dominated by internally produced algal biomass, the C/DW ratio of ~0.4 g C/g DW is comparable to that of fresh algae. In an oligotrophic waterbody, or a free-flowing stream or river, suspended solids can be dominated by inorganic materials with the C/DW ratio ranging from ~ 0.001 to 0.1 g C/g DW (see Chapra, 1997).

In addition to whether or not a sediment transport model allows for the representation of one, or more, classes of cohesive and non-cohesive solids, it is also important to differentiate sediment transport models by their representation of suspended solids as a mixture of inorganic solids and particulate organic matter. Sediment transport models typically do not explicitly represent particulate organic matter as a state variable that is governed by (*a*) external sources from watershed runoff and point source discharges and (*b*) internal sources and sinks from biological processes. For biologically productive water bodies, the internal production of particulate organic carbon can be a factor in the fate of toxic chemicals by sorption of the toxicant with the organic carbon pool derived from biological activity.

*Comparison S2: Representation of Solids Deposition and Resuspension*. In order to satisfy the first-tier screening criteria, a sediment transport model had to differentiate the downward deposition flux of solids from the upward resuspension flux of particles from erosion of the bed. Models are available to specify deposition and resuspension velocities for each particle size class of the model. The key difference between an intermediate model and an advanced sediment transport model is how deposition and resuspension velocities are specified for each particle class. In an intermediate model, the deposition and resuspension velocities are externally provided as data input to the model. With the selection of an intermediate level model, the modeling team calibrates the model using the deposition and resuspension velocities as the adjustable parameters for the model. In an advanced model, the deposition and resuspension velocities are internally simulated using formulations dependent on the basic physical properties and characteristics of each particle class of either cohesive or non-cohesive solids. In a complex model, the adjustable parameters are defined by measurable properties such as the median particle diameter, particle density and the critical stress for resuspension. A complex model actually has fewer degrees of freedom available for model calibration than does an intermediate level model, since the parameter values for deposition and resuspension in a complex model are based on fundamental process formulations rather than simply adjusting the parameter values assigned for deposition and resuspension to obtain the best match to an observed data set.

*Comparison S3: Representation of Cohesive Solids.* An advanced sediment transport model should represent multiple classes of cohesive solids. Solids settling, deposition and resuspension processes should be internally computed in the model using formulations dependent on coupled hydrodynamic model results and the physical properties assigned to each cohesive solids class. Settling velocity is dependent on the concentration of suspended cohesive solids and hydrodynamic conditions (e.g., shear stress, turbulent mixing). Cohesive deposition is dependent on near bed sediment concentration, particle settling velocity and fluid shear stress. Cohesive resuspension is dependent on near bed fluid shear stress and sediment bed properties such as bulk density, shear strength and the fraction of cohesive sediments in the bed.

*Comparison S4: Representation of Non-Cohesive Solids.* An advanced sediment transport model should represent multiple classes of non-cohesive solids. As with cohesive materials, solids settling, deposition and resuspension processes should be internally computed in the sediment transport model using formulations dependent on hydrodynamics and physical properties assigned to each non-cohesive solids class. Settling velocity should be dependent on the discrete particle diameter at low solids concentrations. The net vertical flux from non-cohesive solids deposition and resuspension should be controlled by the near bed sediment concentration, particle settling velocity, bed shear stress, and particle density. Additional parameters that should be calculated in the non-cohesive solids model include the critical Shields parameter and the near bed equilibrium sediment concentration.

*Comparison S5: Representation of Bed Load Transport.* In site-specific cases where bed load transport is identified by the 'conceptual model' as an important process for the mass balance of non-cohesive solids, that in turn influences the transport and fate of the toxic chemicals of concern, the sediment transport model should include the capability to represent bed load transport of non-cohesive solids. The transport of bed load solids by sliding, rolling, and saltation should be controlled in the model by near bottom velocity, particle size and particle density.

Comparison S6: Representation of Surface and Deep Sediment Bed. Sediment transport models can represent coupling of the water column with only a single sediment bed layer or with multiple bed layers. In a sediment transport model, the space and time distribution of solids in the surface layer of the sediment bed must be able to be simulated to allow for the mass balance representation of the deposition of solids to the bed and the upward flux of solids to the water column under bed stress conditions that result in erosion of the bed. Sediment bed models are differentiated by their capability to represent bed armoring of non-cohesive solids and the methods used to simulate: (*a*) solids concentration in the bed surface and deep bed layers; (*b*) thickness of surface layer and deep bed layers; and (*c*) bed consolidation of surface and deep bed layers.

The sediment transport model should be able to represent sediment bed mechanics for a surficial sediment bed with specification of multiple deep bed layers. The thicknesses and geomechanical properties (e.g., void ratio, bulk density, porosity) of each bed layer should be time and space dependent to dynamically account for the mass of solids either deposited to, or eroded from, the surficial bed and consolidation of all layers. The spatial variation of the thickness of the surface sediment bed layer should be able to be assigned using site-specific observations. Spatially variable specifications of sediment bed properties, such as bulk density, porosity or void ratio, should also be able to be defined as input to an advanced sediment bed model.

*Comparison S7: Coupling of Hydrodynamic Model and Sediment Transport Model for Advective and Dispersive Mass Transport.* The sediment transport model must be able to be coupled with the results of a hydrodynamic model to specify the spatial and temporal dependency of water column velocity fields, surface elevation and depth of the water column. These data are needed as input to the advection and turbulent mixing components of the sediment transport model. The spatial resolution of the sediment transport model grid should be either identical to the resolution of the hydrodynamic grid or aggregated to a resolution capable of representing the observed spatial gradients of solids deposition and erosion in the waterbody. The sediment transport model can be structured to allow for either the external linkage of the results of a hydrodynamic model or the internal interface of the sediment transport model and the hydrodynamic model in a single code model framework.

*Comparison S8: Coupling of Hydrodynamic Model and Sediment Transport Model for Deposition and Resuspension Fluxes.* In addition to the interface of velocity fields simulated by a hydrodynamic model for the simulation of the mass transport of solids by advection and dispersion, the results of a hydrodynamic model can also be coupled with a sediment transport model to provide bed shear stresses needed for the computation of deposition and resuspension velocities and the corresponding fluxes of solids.

*Comparison S9: Coupling of Hydrodynamic Model and Sediment Transport Model for Interface of Bathymetry.* In order to rigorously couple simulated velocities and bed shear stresses computed in the hydrodynamic model with simulated changes in surface bed elevation computed in the sediment transport model, the most advanced sediment transport models provide for the internal coupling of changes in water column depth with the numerical solution of the hydrodynamic model.

*Comparison S10: Wetting and Drying and Particle Trapping in a Sediment Transport Model.* Where the ‘conceptual model’ indicates that wetting and drying must be considered as an important physical process of the site-specific waterbody, the export of solids, and any associated adsorbed contaminants, from the natural water system to an adjacent floodplain, wetland, or marsh during periodic wetting and drying events, can be important pathways for the fate of a toxicant as a result of ‘particle trapping’. Particle trapping refers to the physical process wherein solids transported onto the floodplain during out-of-bank flow events remain deposited on the soils and vegetation of the floodplain when the flood flow recedes back into the river channel. The deposition and resuspension formulations of an advanced sediment transport model should be able to account for the effect of particle “trapping” on vegetation in the domain influenced by periodic wetting and drying.

The sediment transport models selected for review and evaluation include the following:

ECOMSED V1.3 and SEDZL
EFDC and EFDC1D
HSCTM-2D V1.0
HSPF-RCHRES V12.0
IPX V2.7.4
WASP5-TOXI5 V5.10 and WASP6-TOXI6 V6.1

Table 3.1 presents a comparison of the state variables adopted for each model. Table 3.2 presents a comparison of the sediment transport processes and interactions incorporated in each model.

Intermediate Models. IPX, WASP5-TOXI5 and WASP6-TOXI6 are all “cousin” models that have been developed by the U.S. Environmental Protection Agency (Ambrose et al., 1988, 1993; Wool et al., 2002) and the Wisconsin Department of Natural Resources (Velleux et al., 2001) using the WASP model framework originally developed by Hydro Qual, Inc. during the 1980's (Di Toro et al, 1983). The sediment transport modules of WASP5, WASP6 and IPX allow for the simulation of up to three classes of “generalized solids” as suspended material. Since solids in the intermediate level of sediment transport model are considered “generalized”, there are no functional relationships included in these models that allow the modeler to differentiate any of the solids classes as cohesive, non-cohesive, inorganic or organic solids. In natural waters, suspended solids, derived from external watershed runoff, internal biological production and decomposition processes, and internal settling, deposition and erosion processes, are comprised of both inorganic solids and detrital and living organic matter. Particulate organic matter (and particulate organic carbon) is not explicitly represented as a solids class in an intermediate sediment transport model. Using site-specific field data, or best estimates from the technical literature, the organic content of suspended solids is represented by the space and time dependency of the organic carbon fraction of suspended solids. The distribution of organic matter, which is crucial for the simulation of the partitioning of a toxicant with solids, is empirically defined in the WASP class of model by the parameterization of the organic carbon fraction of suspended solids. Since non-cohesive solids are not explicitly represented in the intermediate class of models, bedload transport of coarse, non-cohesive material is not considered in these intermediate models.

The WASP class of models is considered an intermediate level sediment transport model primarily because the methodology used to compute the settling of solids within the water column and the exchange of solids between the water column and the sediment bed is based on the external specification of input data to define the mass flux of solids that result from solids settling within the water column and bottom stress conditions and sediment bed properties that may favor either deposition or resuspension of solids. Advanced sediment transport models, by contrast, are based on a dynamic simulation of the mass flux exchange of solids between the water column and the bed where the mass flux exchange of solids is functionally dependent on hydrodynamics, sediment bed properties, solids properties and fluid stresses at the bed-water interface. In the intermediate class of model, the modeler must externally assign parameter values as input data to define the time and space dependency of the settling, deposition and resuspension velocities for each of the three generalized solids classes. Settling, deposition and resuspension parameter values are assigned as input to the intermediate class of model on the basis of: (*a*) site-specific field measurements of settling, deposition and erosion properties of

**Table 3.1. Comparison of Sediment Transport Model State Variables**

| | 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) |
|---|---|---|---|---|---|---|
| SOLIDS CLASSES (SIZE FRACTIONS) | | | | | | |
| Single class | | | | | | |
| Single Generalized Class | | | | | | |
| Single Cohesive Class | ★ | | | | | |
| Single Non-Cohesive Class | ★ | | | ★ | | |
| Multiple classes | | | | | | |
| Multiple Generalized Classes | | | | | ★ | ★ |
| Multiple Cohesive Classes | | ★ | ★ | ★ | | |
| Multiple Non-Cohesive Classes | | ★ | | | | |
| SOLIDS TYPES | | | | | | |
| Inorganics | | | | | | |
| Silt (explicitly defined) | | | ★ | ★ | | |
| Clay (explicitly defined) | | | ★ | ★ | | |
| Sand (explicitly defined) | | | | ★ | | |
| Represented as [1 - Fraction of Organic Carbon (Foc)] * Solids Concentration[1] | ★ | ★ | | | ★ | ★ |
| Organics | | | | | | |
| Represented as Fraction of Organic Carbon (Foc) * Solids Concentration[1] | ★ | ★ | | | ★ | ★ |
| Particulate Organic Matter (POM) or Carbon (POC) | ★ | ★ | | | | |

**footnotes**

**1** In models that use this approach, solids are neither organic nor inorganic material; the fraction of organic carbon (Foc) is assigned to represent organic matter for toxcant partitioning; thus inorganic matter is defined as [1 - Foc]

solids; (*b*) data taken from the technical literature with subsequent calibration to the field data sets obtained for a site-specific problem setting; or (*c*) linkage with simulated values of settling, deposition and resuspension velocities generated by a coupled hydrodynamic and sediment transport model.

Intermediate sediment transport models allow the modeler to specify the vertical distribution of solids in the sediment bed as either: (a) a single surficial sediment bed layer or (b) as a surficial bed underlain by multiple sediment bed layers. In addition to the approach used to define solids deposition and erosion velocities, another key difference between intermediate and advanced sediment transport models is the approach used to account for the coupled interaction of solids deposition and erosion and consolidation of the sediment bed. As solids material is deposited to the bed, or as material is eroded from the bed, the thickness, solids concentration and void ratio, or porosity, of the sediment bed changes over time. The screening level model approach simply assumes that the bed thickness, solids concentration and the void ratio of the bed do not change over time. The mass flux of material across the bed-water interface is thus assumed to describe the mass flux of material across each sediment bed layer. In the intermediate WASP class of sediment transport model, the bed layer thickness (and volume) can be assumed constant

**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

| Table 3.2. Sediment Transport Model Processes (concluded) | 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) |
|---|---|---|---|---|---|---|
| BED FORMATION | | | | | | |
| Surface and Deep Sediment Bed | | | | | | |
| Single Surficial Bed Layer | | | | ★ | | |
| Surficial & Multiple Bed Layers | ★ | ★ | ★ | | ★ | ★ |
| Armoring of Non-Cohesive Bed | | | | | | |
| Not represented | | | | ★ | ★ | ★ |
| Represented in model | ★ | ★ | | | | |
| Bed Solids Concentration | | | | | | |
| Constant in Time | | | | ★ | ★ | ★ |
| Variable in Time (Simulated) | ★ | ★ | ★ | | ★ | ★ |
| Thickness of Bed Layers | | | | | | |
| Constant in Time | | | ★ | ★ | ★ | ★ |
| Variable in Time (Simulated) | ★ | ★ | | ★ | ★ | ★ |
| Bed Consolidation | | | | | | |
| Bed Consolidation Constant in Time | | | | | | ★ |
| Bed Consolidation Represented as Semi-Empirical Time Function | ★ | ★ | ★ | | ★ | |
| Bed Consolidation Represented as Semi-Empirical Depth Function | | ★ | | | | |
| Bed Consolidation Variable in Time (Simulated) | | ★ | | | | |
| Deep SubSurface Bed Layers | | | | | | |
| Number of Deep Subsurface Layers Constant in Time | | | | | | ★ |
| Number of Deep Subsurface Layers Variable in Time (Simulated) | | ★ | ★ | | ★ | |
| Sediment Transport & Hydrodynamic Model Coupling | | | | | | |
| Internal Computation of All Advective and Dispersive Transport Variables | ★ | ★ | ★ | ★ | | |
| Coupling with Externally Provided Advective and Dispersive Transport Variables | | | | | ★ | ★ |
| Internal Computation of All Deposition and Resuspension Variables | ★ | ★ | ★ | ★ | | |
| Coupling with Externally Provided Deposition and Resuspension Variables | | | | | ★ | ★ |
| Internal Coupling of Water/Sediment Bathymetry | ★ | ★ | ★ | | | |
| Feedback Between External Hydrodynamic and Internal Sediment Bathymetry | | ★ | ★ | | | |
| Internal Coupling of Sediment Trapping with Wetting/Drying | | ★ | | | | |
| Coupling of External Wetting/Drying with Sediment Trapping | | | | | | |

over time with the void ratio and solids concentration allowed to change over time because of the input of a "burial velocity" to enable solids mass to continuously move in a downward direction on a "conveyor belt" towards the bedrock or hard pan layer. As an optional approach, the intermediate WASP class of model also allows the surficial bed layer thickness (and volume) to be time-variable while the void ratio, solids concentration and the deep bed layer thicknesses (and volumes) are assumed to be constant over time. Consolidation is empirically represented in the WASP class of intermediate sediment transport models with a user-defined 'sedimentation time step interval' that is much larger than the time step used for numerical integration of the model. As solids are deposited onto the bed, the thickness of the surficial bed continues to increase until the end of the periodic cycle defined by the sedimentation time step interval.  At that time, the thickness of the bed is considered to be consolidated and the density of the surface bed is assigned a value to match the density of the subsurface bed layer.

Although IPX is a WASP “cousin”, the methodology used to represent the time variable change in bed thickness, solids concentration and void ratio is distinctly different between WASP5-TOXI5, WASP6-TOXI6 and IPX Version 2.7.4.  WASP5 and WASP6 adopt the level of the sediment bed-water interface as an Eulerian frame of reference to track the accumulation or erosion of solids in the bed.  With the Eulerian frame of reference used in WASP5 and WASP6, toxicant mass can be erroneously imported from a non-zero toxicant boundary condition for the bottom of the deep bed as an infinite source term (Velleux et al., 2001).  IPX Version 2.7.4, by contrast, uses a Lagrangian frame of reference where the changes in bed layer thickness and solids concentrations are computed in relation to a fixed “hard-pan” elevation defined for the bottom boundary of the sediment bed.  With the Lagrangian scheme adopted in IPX, toxicant mass can never be erroneously exported, or imported, across the bottom boundary of the sediment bed into the domain of the sediment bed (Velleux et al., 2001).

Advanced Models.  ECOMSED and SEDZL, EFDC and EFDC1D, HSCTM-2D and HSPF-RCHRES are all considered advanced sediment transport models.  These models are classified as advanced models for the following three reasons: (1) hydrodynamic and/or hydraulic models are coupled with the sediment transport model to provide bottom stress data as input to the deposition and resuspension sub-models; (2) cohesive and/or non-cohesive solids are explicitly represented as state variables; and (3) the mass flux rates controlling the deposition and resuspension of solids are internally simulated using (*a*) bottom stresses simulated with a coupled hydrodynamic/hydraulic model and (*b*) functional relationships for deposition and erosion  based on fluid stress and solids properties, including critical stresses that either induce solids deposition or trigger resuspension events.  These advanced models explicitly represent cohesive and/or non-cohesive solids with functional relationships used to describe the deposition and erosion properties of cohesive and/or non-cohesive solids based on either laboratory and/or site-specific experiments designed to identify the critical stresses needed to trigger erosion of the sediment bed.  In contrast to the advanced sediment transport formulations used in ECOMSED, EFDC and HSCTM-2D that have been taken from the literature published during the past 10-15 years, the sediment transport formulations used in HSPF-RCHRES are based on literature published during the 1960s and 1970s.  As a remedy for the calibration problems that have been attributed to the out-dated formulations used in HSPF-RCHRES, Ziegler and Owen (2001) have proposed that the advanced sediment transport formulations used in ECOMSED and SEDZL (Ziegler et al., 1990; Ziegler and Nisbet, 1994) be incorporated in a modified version of HSPF.  EFDC1D (Hamrick, 2001; Hayter et al., 2001) was originally developed to enable external linkage of HSPF to a true hydrodynamic model with upgraded sediment transport formulations.

Cohesive and non-cohesive classes of solids can both be simulated in ECOMSED (SEDZL) and EFDC (EFDC1D). ECOMSED (and SEDZL) allows for a single class of cohesive solids and a single class of non-cohesive solids while EFDC (and EFDC1D) allows for the simulation of multiple size-fraction classes of both cohesive and non-cohesive solids.  Similar to EFDC, HSTCM-2D is designed to allow for the simulation of multiple classes of cohesive solids. Non-cohesive solids, however, are not simulated in HSTCM-2D since this model was originally developed and applied for estuarine problem settings characterized by cohesive mud.  HSPF-

RCHRES allows for the simulation of two classes of cohesive solids with standard size fractions of solids assigned as inorganic “clays” and “silts”. A single class of non-cohesive solids is assigned in HSPF-RCHRES as “sands”. Particulate organic matter (POM) is empirically represented in ECOMSED and EFDC using a time and space parameterization of the suspended solids fraction of organic carbon. In HSPF-RCHRES, POM is implicitly included as a component of carbonaceous biochemical oxygen demand (CBOD). POM is not represented in the sediment transport model since the particulate fraction of CBOD is deposited to the sediment bed via a simple net settling velocity. It is noted that none of these advanced models incorporate POM as an explicit solids state variable with deposition and erosion of POM controlled by cohesive solids properties typically associated with organically enriched silty materials.

As with the intermediate models, advanced sediment transport models allow the modeler to specify the vertical distribution of solids in the sediment bed as either: (*a*) single surficial sediment bed layer or (*b*) as a surficial bed underlain by multiple deep sediment bed layers. In contrast to ECOMSED, EFDC and HSCTM-2D where multiple bed layers can be simulated, HSPF-RCHRES is limited to a single surficial sediment bed to represent the exchange of solids and toxicants between the bed and the water column. Advanced sediment transport models typically represent the coupled interaction of solids deposition and erosion and the dynamic consolidation of the sediment bed. ECOMSED, EFDC and HSCTM-2D employ semi-empirical time functions to describe bed consolidation processes. EFDC is the only advanced model that allows the options of semi-empirical depth dependent functions and fully time variable consolidation sub-model to be used to describe bed consolidation. HSPF-RCHRES does not represent either bed consolidation or bed armoring since the HSPF sediment bed is defined only by a surficial bed. Armoring of a non-cohesive sediment bed is included in ECOMSED and EFDC. Since HSCTM-2D represents only cohesive solids, armoring of the non-cohesive bed is not included as a process in the resuspension sub-model.

Over a period of time, the depth and velocity of a depositional reach of a river will decrease as a result of the accumulation of solids in the bed. Unlike ECOMSED and HSPF-RCHRES, EFDC and HSCTM-2D are designed to couple changes in water column depth with changes in bed thickness as dynamically changing feedback for the bathymetry data used as input to the hydrodynamic model. The hydrodynamic models of EFDC and HSCTM-2D represent periodic wetting and drying of portions of the model domain (e.g., floodplains or tide flat areas). The sediment transport components of EFDC and HSCTM-2D also internally account for sediment trapping in wetting and drying areas via deposition of solids to the bed during periods of inundation.

### 3.2.2 Toxic Chemical Transport and Fate Models

Toxic chemical fate models have been developed to represent a number of physical-chemical kinetic processes including the adsorption and desorption of a toxicant with solids and organic matter. Because of the interaction of toxic chemicals with organic matter and suspended sediments, chemical fate models are designed to explicitly account for the interaction of solids with partitioning of the toxicant in the water column and sediment bed. The coupling of a well-developed hydrodynamic and sediment transport model with a toxic chemical transport and fate model for natural water systems is the key component of a model framework for toxic chemicals that can be used to evaluate risk management scenarios based on the effectiveness of alternative remediation strategies. Toxic chemicals include three categories: (1) synthetic organic chemicals (e.g., PCBs, DDT, chlorinated hydrocarbons, PAHs); (2) radionuclides (cesium, strontium etc); and (3) heavy metals (lead, iron, zinc, mercury, cadmium etc).

As is typical for all categories of surface water models, toxic chemical transport and fate models have been developed over the past few decades as very simplified screening level models, intermediate level models applied for water quality management planning studies, and complex, or advanced, models developed for R&D studies and applied problem settings characterized by complex physical domains and a need for a high level of scientific credibility.

Screening level toxic chemical models are designed for very simplified, steady-state, idealized spatial representations of transport and exchange within a one-dimensional waterbody. These simplified models, usually derived as analytical solutions, typically account for only a single point source wastewater discharge, a single chemical and a single class of suspended solids. The kinetics of screening level models are usually simplified to account only for an overall loss of a toxic chemical from the water column. The loss rate of the toxic chemical is typically parameterized as an "effective" first-order loss rate based on settling of the sorbed toxicant and a composite sum of the losses resulting from other physical-chemical processes and interactions (e.g., volatilization). The mass of the toxic chemical available in the sediment bed is not represented in this type of a simple model. Screening level models are too simplified to be technically acceptable for the purposes of this study.

Intermediate level chemical fate models are designed for steady-state and time-variable conditions, a more realistic spatial representation within a one-, two- or three-dimensional waterbody and the capability to represent multiple point source inputs. Intermediate level models typically represent only one chemical and a single class of suspended solids with exchange allowed between the water column and sediment bed via solids deposition and resuspension and vertical diffusion of the dissolved form of the chemical. Kinetic reaction terms of an intermediate model include chemical partitioning and one, or more, other physical-chemical processes with each kinetic term defined as a separate process. Rate reactions and other parameters are obtained from external data sources and provided as input to the model. Intermediate-level chemical fate models can represent the distribution of the total, dissolved and particulate, forms of a single chemical in both the water column and, at a minimum, the surficial sediment bed.

Advanced or complex level chemical fate models are designed for time-variable conditions that allow for a multi-dimensional spatial representation of a waterbody and the capability to accommodate nonpoint source watershed runoff and multiple point source inputs. Advanced level models can represent multiple chemicals and multiple classes of suspended solids with exchange allowed between the water column and sediment bed via solids deposition and resuspension and vertical diffusion of the dissolved form of the chemical. Kinetic reaction terms of an advanced model include the representation of chemical partitioning with suspended solids and the organic carbon equivalent of solids within the water column and the sediment bed. In addition to chemical partitioning, an advanced model allows for the representation of all the following possible physical-chemical kinetic processes: volatilization, hydrolysis, photolysis, oxidation, and biodegradation. An advanced model *may* also allow for the representation of the kinetic transformation of a toxicant as 'daughter' products by the input of reaction yield information, speciation (of metals), or complexation (of organic chemicals). Rate reactions and other parameters are obtained from external data sources and can be provided as input to the model using different parameter values for the water column and the sediment bed. Advanced chemical fate models allow for the representation of the distribution of the total, dissolved and particulate forms of multiple chemicals in the water column and, at a minimum, the surficial sediment bed.

In reviewing and evaluating the various features or processes of a toxic chemical transport and fate model, the detailed assessment of candidate models focused on (a) the capability of a candidate model to represent a key feature, attribute, process or interaction; and (b) the level of detail of the formulation(s) used to describe the processes or interactions. When the model comparisons are used for selection of a model, the 'conceptual model' of the site-specific problem setting will determine which attributes of the head-to-head comparison are the most relevant.

In comparing the attributes of candidate toxic chemical models, the methods used in each model to represent the following model components were considered:

(1) Toxicant class
(2) Sorption of toxicant
(3) Physical-chemical kinetics
(4) Surficial and deep sediment bed
(5) Additional nonpoint source boundary inputs
(5) Coupling of hydrodynamics, sediment transport and toxic chemical models
(6) Linkage with a bioaccumulation model

*Comparison T1: Representation of Toxicant Class.* Toxic chemical models have been developed to represent the transport and fate of the three general classes of toxicants: (a) synthetic organic chemicals (e.g., PCBs, DDT); (b) radionuclides (e.g., cesium); and (c) heavy metals (e.g., cadmium). Some chemical fate models have been developed specifically for only one of these classes such as EXAMS (Burns, 2002) for heavy metals. Others have been developed as general chemical fate models applicable for all classes of toxicants. The specific problem application and the 'conceptual model' then drives the assignment of parameter values for the different reaction terms applicable to synthetic organic chemicals, radionuclides or heavy metals. Kinetic processes not relevant to a particular chemical are eliminated from a model framework simply by assigning a parameter value of zero to the kinetic term.

*Comparison T2: Sorption of Toxicants.* A key kinetic process influencing the fate of toxic organic chemicals, radionuclides and heavy metals is the physical-chemical affinity of a toxicant to be adsorbed onto solids. Sorption of a toxicant with solids is a major pathway for the transport of toxic chemicals in natural waters since the toxicants are distributed, and redistributed, by the transport of sediments through the aquatic ecosystem by settling, incorporation of a toxicant into the sediment bed and resuspension of sorbed toxicants under high bottom stress conditions. The long-term interaction between the dissolved and particulate states of the toxicant leads to a condition of dynamic equilibrium. The equilibrium condition, assumed to be "instantaneous", between the dissolved concentration of a toxicant and the mass concentration of solids is then defined in accordance with the class of toxicant and the type of solids (clays, silts, organic matter) that adsorb the toxicant as a partition coefficient.

For many 'neutral' synthetic organic chemicals, hydrophobic effects cause the toxicant to associate with organic matter in the particulate phase. In addition to the well-known affinity for sorption onto organic matter, synthetic organic chemicals can also be sorbed to inorganic solids such as clays when the organic content of particulate matter is very low. Radionuclides, similar to toxic organic chemicals, also are sorbed onto organic matter and fine-grained inorganic solids such as clays. Sorption of heavy metals differs from sorption of synthetic organic chemicals. Metals can first be complexed by organic ligands and then sorbed to organic matter in a manner similar to toxic organic chemicals. Physical adsorption to solid surfaces, chemical sorption or binding by ligands and ion exchange are additional physical-chemical processes that must be considered in formulations describing the sorption of metals onto solids. In addition to sorption, heavy metals can be transformed by speciation into different chemical forms that, in turn, can exhibit differences in transport, fate and toxicity (Chapra, 1997).

Toxic chemical fate models can be differentiated by the methodologies adopted to represent either two-phase or three-phase partitioning of a toxicant. The simplest chemical fate model defines the two-phase partitioning of the total concentration of a toxicant as the sum of the dissolved and particulate fractions. The partition coefficient is defined as a 'distribution' coefficient [$K_d$] in terms of the total suspended solids concentration. The 'distribution' coefficient and the suspended solids concentration then combine to define the dissolved fraction of the toxicant. For neutral, organic chemicals, the two-phase partition model can be somewhat more complex by specifying the partition coefficient on the basis of the particulate organic carbon content of the solids [$f_{oc}$] (i.e., carbon to dry weight ratio) and an organic carbon-based partition coefficient [$K_{oc}$]. The organic carbon-based partition coefficient, in turn, can be defined by the toxicant's octanol-water partition coefficient [$K_{ow}$]. The most complete description of chemical partitioning is a three-phase model where the toxicant is partitioned into three forms as a truly dissolved (bio-available) phase, a dissolved organic carbon phase (not bio-available) and a particulate organic carbon phase. A three-phase model is most appropriate for natural waters characterized by a significant proportion of solids that are derived from internally produced organic matter from biological processes in contrast to externally supplied solids from watershed runoff and point source discharges.

Chemical fate models are thus differentiated by the use of either two-phase or three-phase formulations for the representation of the sorption of a toxicant. Models are further differentiated by the definition of the partition coefficient as either a solids-based 'distribution' coefficient [$K_d$] or an organic carbon-based partition coefficient [$K_{oc}$]. Ideally, the model should allow for the optional input of the partition coefficients using either a (1) suspended solids basis for the distribution coefficient ($K_d$); or a (2) particulate organic carbon basis for the organic carbon normalized partition coefficient ($K_{oc}$). Models are also differentiated by whether or not a chemical fate model allows for the assignment of different partition coefficients and fractions of organic carbon [$f_{oc}$] for the water column and the sediment bed. Finally, if the model provides for a three-phase partition formulation, the chemical fate model should allow for the coupling of time and space distributions of dissolved organic carbon (DOC) for three-phase partitioning of the toxicant. The distribution of DOC can be provided in two ways to a toxic chemical fate model. DOC can be provided by the user as externally specified input data to the model or DOC can be internally simulated with a biological model and coupled with the toxic chemical fate model.

The sediment transport model and the toxic chemical fate model should be structured to explicitly account for a total solids mass balance of inorganic solids and particulate organic matter. In determining what forms of solids need to be incorporated in the model framework, the site-specific 'conceptual model' should provide quantitative information about the relative mass loading contributions of the sources and sinks of inorganic solids and organic matter derived from: (*a*) external sources from watershed runoff, tributaries and point source discharges; and (*b*) internal sources from *in situ* biological processes of organic matter production and decomposition, and physical processes of particle deposition and resuspension. For a waterbody characterized by relatively high loading of organic solids derived from internal biological activity (e.g., eutrophic or nutrient enriched waterbodies), the chemical fate model should allow for the coupling of time and space distributions of particulate organic carbon (POC) for organic carbon-based partitioning of the toxicant. The distribution of POC can be provided in two ways to a toxic chemical fate model. POC can be provided by the user as externally specified input data to the model, or POC can be internally simulated as living (algae) POC and non-living detrital POC with a biological model and coupled with the toxic chemical fate model. Note that if POC is explicitly interfaced with a chemical fate model, then the fraction of organic carbon [$f_{oc}$] is determined by the model, rather than specified as input data to the model, as the carbon to dry weight ratio of POC to TSS, where the TSS must include the inorganic solids and the particulate organic matter (POM) dry weight equivalent of POC.

*Comparison T3: Physical-Chemical Kinetics.* In addition to sorption and desorption, physical and biogeochemical processes typically represented in chemical fate models also include: chemical hydrolysis, photolysis, volatilization, microbial degradation, biological transformations, and chemical oxidation. Speciation of heavy metals, complexation of organic chemicals, and parent-daughter chemical relationships *may* also be represented. Chemical fate models can be differentiated by the level of detail used in the formulations for each of these kinetic processes.

*Comparison T4: Representation of Surficial and Deep Sediment Bed.* Toxic chemical models can represent coupling of the water column with (a) only a surficial sediment bed or with (b) multiple bed layers. In a toxic chemical model, the space and time distribution of toxicant in the surficial sediment bed must be able to be simulated to allow for the mass balance representation of the deposition of sorbed toxicant to the bed and the upward flux of sorbed toxicant to the water column from erosion of the bed. The toxic chemical fate model should be able to represent spatial and temporal variation of the concentration of the total chemical in the surficial sediment bed and multiple deep bed layers.

The thickness of the surficial bed layer defined for the sediment transport and chemical fate models should be based on observations of “active layer” depths that reflect site-specific rates of biological mixing (bioturbation). The thickness of each layer of the sediment bed model should also be specified to be consistent with site-specific net sediment accumulation rates and the related “memory” time scale of the sediment bed to resolve decadal time scales needed to simulate the chronology of: (*a*) the cumulative contamination of a sediment bed because of historical releases of the toxicant; and (*b*) time scale required for recovery of the sediment bed contamination in the evaluations of alternative remediation strategies. The thickness of the deep bed layers assigned in the sediment transport and chemical fate models should also be consistent with the vertical resolution of contaminant concentrations from site-specific sediment core records.

The vertical transport of the dissolved form of the toxicant between the sediment bed and the overlying water column should be able to be represented by porewater transport processes of advection and diffusion. Vertical transport of the sorbed fraction of the chemical contaminant within the sediment bed should be able to be represented by vertical mixing of the solids between bed layers resulting from bioturbation. Vertical exchange of the dissolved form of the chemical computed from the vertical gradient of water column and porewater dissolved chemical concentrations should be consistent with the vertical advection of porewater that is dependent on changes in sediment bed porosity, void ratio or bulk density.

*Comparison T5: Additional Nonpoint Source Boundary Inputs.* For chemical fate models, atmospheric deposition and distributed inflow from leachate fields of hazardous waste sites and contaminated groundwater can also serve as external sources of toxic chemicals to a waterbody. If the 'conceptual model' indicates that these sources are significant for a site-specific problem setting, then the chemical fate model should be capable of representing these distributed sources of toxicant into the physical domain of the model.

*Comparison T6: Coupling of Hydrodynamic Model and Sediment Transport Model with Toxic Chemical Fate Model for Advective and Dispersive Mass Transport.* The toxic chemical transport and fate model must be able to be coupled with the results of a hydrodynamic model and sediment transport model to specify the spatial and temporal dependency of velocity fields, depth of the water column, and concentration distributions of cohesive and non-cohesive solids in the water column and sediment bed. These data are needed as input to the transport and fate components of the toxicant model. The spatial resolution of the toxic model grid should either be identical to the resolution of the hydrodynamic grid or aggregated to a coarser resolution identical to the resolution of the sediment transport model. The toxic chemical model can be structured to allow for either the external linkage of the results of a hydrodynamic and sediment transport model or the internal interface of the toxic chemical model and the hydrodynamic model and sediment transport model in a single code model framework.

*Comparison T7: Coupling of Toxic Chemical Fate Model with Bioaccumulation Model.* The results of the chemical fate model should be able to be linked as input to a toxic chemical bioaccumulation model for risk assessment simulations. Spatially dependent time series of the exposure concentrations of the dissolved and sorbed forms of the contaminant in the water column and sediment bed should be able to be linked as input data to a bioaccumulation model. Sorbed chemical concentrations should be able to be normalized to particulate organic carbon concentrations in the water column and sediment bed of the waterbody for linkage of the results of the chemical fate model with a bioaccumulation model.

The toxic chemical transport and fate models selected for review and evaluation include the following models:

AQUATOX V2.0
EFDC and EFDC1D
HSCTM-2D V1.0
HSPF-RCHRES V12.0
IPX V2.7.4
WASP5-TOXI5 V5.10 and WASP6-TOXI6 V6.1

Table 3.3 presents a comparison of the state variables, kinetic processes and features incorporated in each model.

Intermediate Models. None of the models selected for review and evaluation are considered to be intermediate toxic chemical models. The intermediate toxics models considered in this study (see Appendix A) were eliminated during our initial screening of models.

Advanced Models. AQUATOX, EFDC and EFDC1D, HSCTM-2D and HSPF-RCHRES, IPX and WASP5-TOXI5 and WASP6-TOXI6 are all considered advanced toxic chemical transport and fate models. These models are classified as advanced models for the following reasons: (1) the models allow for multi-dimensional spatial representations of a waterbody; (2) the models allow for the simulation of multiple toxicants that can interact with multiple classes of solids; (3) the models allow for partitioning of a toxicant to solids; and (4) the models explicitly represent physical-chemical kinetic processes (e.g., photolysis, hydrolysis and volatilization). EFDC and EFDC1D, IPX, WASP5-TOXI5 and WASP6-TOXI6 are designed to represent multiple generalized toxicants rather than specific classes of a toxicant such as synthetic organic chemicals, radionuclides or heavy metals. Although IPX, WASP5-TOXI5 and WASP6-TOXI6 are "cousins", IPX has been modified by Velleux et al. (2001) to allow the modeler the flexibility to simulate multiple chemicals rather than the maximum limitation of only three chemicals in the WASP5-TOXI5 and WASP6-TOXI6 models. The assignment of the specific values selected to represent the kinetic parameters then defines the specific toxic chemical represented in these models. AQUATOX, by contrast, is designed to account for up to 20 generalized organic chemicals; the assignment of the kinetic parameters defines the specific organic chemical (e.g., PCBs, DDT etc.) represented in the model. Heavy metals and radionuclides are not represented in AQUATOX. HSCTM-2D is designed specifically for multiple generalized heavy metals; the assignment of kinetic parameters defines the specific heavy metal (e.g., copper, lead, zinc, etc.).

Partitioning of many toxicants with solids is a major pathway that can control the transport and fate of a toxicant within the water column, the sediment bed, adjacent floodplain and riverbanks. Adsorption and desorption of heavy metals can be described using a "2 phase partitioning model" where the solids concentration and a "distribution coefficient (Kd)" are required to simulate the partitioning of a heavy metal between the dissolved and particulate phases. HSCTM-2D, designed specifically to represent heavy metals, allows only for 2 phase partitioning of a heavy metal with solids. HSPF-RCHRES, designed to represent multiple generalized toxicants, also allows only 2 phase partitioning of a toxicant with solids in the water column and bed. Two phase partition models can also be used to simulate sorption of a synthetic organic chemical using the "organic carbon-based partition coefficient, Koc" and the organic carbon fraction of solids. EFDC and EFDC1D, IPX and WASP5-TOXI5 and WASP6-TOXI6 allow the modeler to simulate 2 phase partitioning of a generalized toxicant using either Kd (solids distribution coefficient) or Koc (organic carbon-based partition coefficient). The most complete specification for organic carbon-based partitioning of an organic chemical requires a 3 phase model where the toxicant is partitioned into 3 phases as (1) dissolved (available); (2) DOC-sorbed (unavailable); and (3) particulate forms. AQUATOX is designed to model 3 phase partitioning of an organic chemical on an organic carbon basis. EFDC and EFDC1D, IPX and WASP5-TOXI5 and WASP6-TOXI6 allow the modeler to assign the kinetic parameters for sorption so that either a 2 phase or a 3 phase model can be selected to represent partitioning of a generalized toxicant. Of these advanced models, HSCTM-2D is the only model that does not allow the specification of different kinetic partition coefficients for the water column and the sediment bed.

For AQUATOX, EFDC and EFDC1D, IPX and WASP5-TOXI5 and WASP6-TOXI6, the advanced toxics models designed to represent partitioning of a toxicant with organic carbon, the distribution of particulate organic carbon (POC) is needed for the 2 phase and the 3 phase models. For the 3 phase model available in these advanced models, the distribution of dissolved organic carbon (DOC) is also needed to compute the DOC-sorbed fraction of the toxicant. The organic carbon distributions, in time and space, can be defined for these

**Table 3.3. Toxic Chemical Transport and Fate Model State Variables and Processes**

| | AQUATOX V.2.0 | EFDC & EFDC1D V.1 | HSCTM-2D v.1 | HSPF-RCHRES V.12 | IPX 2.7.4 | WASP5(6)-TOXI5(6) |
|---|---|---|---|---|---|---|
| STATE VARIABLES | | | | | | |
| Toxicant Classes | | | | | | |
| Single Generalized Toxicant | | | | | | |
| Multiple Generalized Toxicants | | ★ | | ★ | ★ | ★ |
| Synthetic Organic Chemicals | 1 | ★ | | | ★ | ★ |
| Radionuclides | | ★ | | | ★ | ★ |
| Heavy metals | | ★ | ★ | | ★ | ★ |
| KINETIC PROCESSES | | | | | | |
| Toxicant Sorption & Desorption | | | | | | |
| Partitioning of Toxicant | | | | | | |
| Two-phase Partitioning-solids Based (Kd, SS, dissolved) | | ★ | ★ | ★ | ★ | ★ |
| Two-phase Partitioning-organic Carbon Based (Koc, POC, dissolved) | | ★ | | | ★ | ★ |
| Three-phase Partitioning-organic Carbon Based (Koc,DOC, POC, dissolved) | ★ | ★ | | | ★ | ★ |
| Allows Assignment of Different Coefficients (Koc or Kd) for Water Column & Sediment Bed | ★ | ★ | | ★ | ★ | ★ |
| Allows Assignment of Different Fractions of Org-C (Foc) for Water Column & Sediment Bed | | ★ | | | ★ | ★ |
| Dissolved Organic Carbon (DOC) | | | | | | |
| Coupling with Time & Space Distributions of DOC for Partitioning of Toxicant | | ★ | | | ★ | ★ |
| Allows Assignment of DOC Data as Input to Model | | ★ | | | ★ | ★ |
| Internally Simulates DOC Using a Biological Model | ★ | 2 | | | | |
| Particulate Organic Carbon (POC) | | | | | | |
| Coupling with Time & Space Distributions of POC for Partitioning of Toxicant | | ★ | | | | |
| Allows Assignment of POC Data as Input to Model | | ★ | | | | |
| Internally Simulates POC Using a Biological Model | ★ | 2 | | | | |
| Physical-Chemical Kinetics | | | | | | |
| Generalized First-order Reaction | | ★ | | ★ | ★ | ★ |
| Hydrolysis | ★ | ★ | | ★ | ★ | ★ |
| Photolysis | ★ | ★ | | ★ | ★ | ★ |
| Volatilization | ★ | ★ | | ★ | ★ | ★ |
| Microbial Degradation | ★ | ★ | | ★ | ★ | ★ |
| Chemical Oxidation | | ★ | | ★ | ★ | ★ |
| Parent/Daughter Transformations for Generalized Toxicants | | | | ★ | ★ | ★ |
| Speciation of Heavy Metals | | | | | | |
| Complexation of Organic Chemicals | | | | | | |

**footnotes**

**1** AQUATOX can model up to 20 organic chemicals simultaneously.

**2** POC and DOC are only simulated if the EFDC eutrophication module is active.

advanced toxics model as either (a) externally specified empirical concentrations of DOC and POC in the water column and sediment bed or (b) internally simulated concentrations of DOC and POC in the water column and bed provided by an internally coupled biological model. EFDC and EFDC1D, IPX, WASP5-TOXI5 and WASP6-TOXI6 all allow the modeler to define externally provided space and time functions that describe empirical distributions of DOC based on site-specific field data as input to these models. In contrast to the "WASP cousins" IPX, WASP5-

| Table 3.3. Toxic Chemical Transport and Fate Models (concluded) | AQUATOX V.2.0 | EFDC & EFDC1D V.1 | HSCTM-2D V.1 | HSPF-RCHRES V.12 | IPX 2.7.4 | WASP5(6)-TOXI5(6) |
|---|---|---|---|---|---|---|
| KINETIC PROCESSES (concluded) | | | | | | |
| Surface and Deep Bed Sediment | | | | | | |
| Single Bed Layer | | | | ★ | | |
| Multiple Bed Layers | ★ | ★ | ★ | | ★ | ★ |
| Time-variable Toxicant Bed Concentrations | ★ | ★ | ★ | ★ | ★ | ★ |
| Space-variable Toxicant Bed Concentrations | | ★ | ★ | ★ | ★ | ★ |
| Advection & Diffusion of Dissolved Toxicants in Porewater | ★ | ★ | | | ★ | ★ |
| Vertical Mixing of Sorbed Toxicants via Bioturbation | | ★ | | | | |
| Nonpoint Source Boundary Inputs | | | | | | |
| Atmospheric Deposition (wet precipitation input) | ★ | ★ | | ★ | | |
| Atmospheric Deposition (dry non-precipitation input) | ★ | ★ | | ★ | | |
| Distributed Flow & Toxics Load from Leachate Fields & Groundwater (lateral input to water) | | ★ | | | ★ | ★ |
| Distributed Flow & Toxics Loads from Groundwater (vertical input to bed) | | ★ | | | | |
| Toxic Chemical Fate Model Coupling with Hydrodynamic Models | | | | | | |
| External Linkage Provided by Hydraulic & Hydrodynamic Flow Variables | ★ | | | ★ | ★ | ★ |
| Internal Coupling with Hydrodynamic Model within a Single Model Framework | | ★ | ★ | 1 | | |
| Toxic Chemical Fate Model Coupling with Sediment Transport Models | | | | | | |
| External Linkage Provided by Sediment Transport Model Variables | ★ | | | | | |
| Internal Coupling with Particulate/Dissolved Organic Matter within a Single Model Framework | ★ | | | | | |
| Internal Coupling with Sediment Transport Model within a Single Model Framework | | ★ | ★ | ★ | ★ | ★ |
| Toxic Chemical Fate Model Coupling with Bioaccumulation Models | | | | | | |
| Internal Coupling with Bioaccumulation Model within a Single Model Framework | ★ | | | | | |
| Dissolved & Sorbed Toxicant Concentrations Available for Export/Linkage | | ★ | | ★ | ★ | ★ |
| **footnotes** | | | | | | |
| 1 Coupling is to a kinematic wave model | | | | | | |

TOXI5 and WASP6-TOXI6, EFDC and EFDC1D also allow a modeler to define externally provided space and time functions that describe empirical distributions of POC based on site-specific field data as model input. IPX, WASP5-TOXI5 and WASP6-TOXI6 use the total suspended solids concentration with the user-assigned fraction of organic carbon (Foc) to compute the POC concentration required for the organic carbon-based 2 phase and 3 phase partition model.

The EFDC model framework includes internally coupled advanced models for hydrodynamics, sediment transport, toxicant fate and conventional water quality, nutrient enrichment and eutrophication. DOC and POC can be readily simulated with activation of the eutrophication model. The results of the biological model are not, however, as of March 2003, internally linked with the toxicant model to provide a coupled distribution of DOC and POC as input to the organic carbon-based 3 phase partition model. EFDC is presently designed to allow the modeler to provide DOC and POC data as externally supplied space/time forcing function data for input to the toxics model. EFDC's biological model does not have to be activated to run the toxics model. The level of effort required to activate the biological model, in addition to the sediment transport and toxicant fate models of EFDC, is substantial. The mass balance credibility of a toxics model framework can be greatly enhanced, however, by activating EFDC's internal biological model if the site-specific 'conceptual model' indicates that (a) the waterbody is biologically enriched (eutrophic) and biologically produced organic matter is a significant component of the solids budget; and/or (b) the alternative remediation actions are expected to result in long-term alterations to the biological productivity of the waterbody (e.g., change in physical regime or change in external loading of nutrients or solids). If the 'conceptual model' suggests that (a) biologically produced organic matter is a minor component of the solids budget and/or (b) if the remediation action is not expected to alter biological production of a waterbody, then it is reasonable to bypass activation of the biological model in EFDC. Under this 'conceptual model', DOC and POC distributions can be appropriately described using externally provided site-specific data as input to the toxicant model.

Unlike EFDC and EFDC1D, IPX and WASP5-TOXI5 and WASP6-TOXI6 where DOC and POC are obtained from externally provided data as input to the toxics model, the internal biological model of AQUATOX is used to simulate the time and space distributions of DOC and POC for internal coupling with the 3 phase partition model for one or more organic chemicals. The biologically simulated concentrations of DOC and POC, driven by production, respiration and decomposition processes, are used to partition an organic chemical into the dissolved, DOC-sorbed and POC-sorbed phases of the toxicant. The body burden of the organic chemical for an organism, determined from the internal bioaccumulation model of AQUATOX, is then coupled with a toxicity sub-model, which in turn, may alter the biological state of the system and result in a change in the distributions of DOC and POC. Because the biological model is an integral component of the toxics model, AQUATOX clearly is the most complex of the advanced toxic chemical models.

In addition to sorption and desorption, the other physical-chemical kinetic processes incorporated in advanced toxicant models include: generalized kinetic reaction, hydrolysis, photolysis, volatilization, microbial degradation, chemical oxidation, chemical transformations, speciation of metals and complexation of organic chemicals.

EFDC and EFDC1D, HSPF-RCHRES, IPX and WASP5-TOXI and WASP6-TOXI6 allow the modeler to define a generic first-order reaction term in addition to the other specific physical-chemical processes. HSPF, IPX, WASP5-TOXI and WASP6-TOXI6 allow the modeler to specify an interaction matrix to define 'parent-daughter' transformations of a toxicant to a different toxicant (e.g., DDE as a metabolite of DDT). With the exception of AQUATOX, all the advanced models represent chemical oxidation. None of the advanced models selected for our evaluation, however, provide the capability to simulate speciation of metals or complexation of organic chemicals. Public domain models are available, however, to provide algorithms, if needed for future model development, for metals speciation (e.g., EXAMS, Burns, 2002) and complexation of organic chemicals (e.g., MINTEQA2, Allison et al., 1991).

The advanced toxic chemical models allow the modeler to specify the vertical distribution of toxic chemicals in the sediment bed as either: (a) single surficial sediment bed layer or (b) as a surficial bed underlain by multiple deep sediment bed layers. In contrast to AQUATOX, EFDC, HSCTM-2D, IPX and WASP5-TOXI5 and WASP6-TOXI6 where multiple bed layers can be simulated, HSPF-RCHRES is limited to a single surficial sediment bed to represent the exchange of toxicants between the sediment bed and the water column.

In contrast to HSCTM-2D and HSPF-RCHRES, AQUATOX, EFDC, IPX, WASP5-TOXI5 and WASP6-TOXI6 are designed to allow for the representation of the vertical exchange of dissolved chemical mass via advection and diffusion within the porewater of the bed. Of the advanced toxics models, EFDC is the only model that can represent the vertical mixing of sorbed toxicants via bioturbation. Unlike models that have been developed specifically to represent bioturbation of toxicants within the sediment bed (see Thoms et al., 1995), bioturbation can be empirically represented, and calibrated, in EFDC by parameterizing the vertical mixing coefficient with an increased value.

Of the advanced toxics models, EFDC and EFDC1D, HSCTM-2D and HSPF-RCHRES incorporate hydrodynamic and/or hydraulic models that allow for an internal interface of flow, velocity and turbulent mixing data as input for the advective and dispersive transport computations. HSPF-RCHRES is the only advanced toxics model that employs a one-dimensional kinematic wave hydraulic model to provide internal flow and velocity data as input to the toxics model. AQUATOX, IPX, WASP5-TOXI5 and WASP6-TOXI6 are all dependent on externally provided transport data for the advective and dispersive mass transport computations. Transport data for these models can be obtained either from (a) site-specific flow balance estimates; or (b) linkage of simulation results provided by an external hydrodynamic and/or hydraulic model.

Since the distribution of solids is a critical element of a toxics model framework, it is important to clearly understand how the advanced toxics models are linked, or coupled, with results generated by a sediment transport model. AQUATOX, EFDC and EFDC1D, HSCTM-2D, HSPF-RCHRES, IPX, WASP5-TOXI5 and WASP6-TOXI6 all are internally coupled with sediment transport models to provide the necessary solids data for the chemical sorption sub-model. The results of external sediment transport models can also be used to provide the linkage for the data needed to describe the distribution of inorganic solids (clays, silts and sands) and particulate organic matter for input to AQUATOX, WASP5-TOXI5 and WASP6-TOXI6. AQUATOX, however, of all the advanced toxics models, is the only model that directly couples simulated distributions of dissolved and particulate organic matter as input to the 3 phase sorption sub-model of the toxics model. AQUATOX is also the only advanced toxics model where the toxicant distributions are directly coupled to an internal bioaccumulation model. The results of the other advanced toxics models (EFDC, HSCTM-2D, IPX and WASP5-TOXI5 and WASP6-TOXI6) can be provided to stand alone bioaccumulation models as externally linked time/space distributions of the dissolved, DOC-sorbed and POC-sorbed forms of a toxicant. WASTOX, for example, included an early version of the WASP toxics model (Connolly and Winfield, 1984) where the chemical exposure results simulated for the water column and bed were linked to the food chain bioaccumulation component of the WASTOX model framework (Connolly and Thomann, 1985).

### 3.2.3 Conventional Pollutant Transport and Fate Models

As is typical for all categories of surface water models, conventional pollutant fate and eutrophication models have been developed over the past few decades as very simplified screening level models, intermediate level models applied for water quality management planning studies, and complex, or advanced, models developed for R&D studies and applied problem settings characterized by complex physical domains and a need for a high level of scientific credibility.

Screening level models of conventional pollutants are typically designed to account only for simplified pathways of chlorides, bacteria, carbon, nutrients and dissolved oxygen in the water column. Some screening level models represent only steady-state conditions in a one-dimensional stream or river. Carbon is represented in screening models as carbonaceous biochemical oxygen demand (CBOD). Nutrients are represented in screening models only as nitrogen. The forms of nitrogen considered in the nitrogen cycle can include nitrogenous BOD (NBOD), organic nitrogen, ammonia, and nitrite + nitrate. The different forms of nitrogen are included in a screening model only to account for the oxygen demand associated with nitrification. The interactions of nutrients and dissolved oxygen with algal photosynthesis and respiration and the interaction of deposited particulate organic carbon and sediment oxygen demand are typically represented empirically in the simplest screening level models as externally provided input data to the model. During the 1970s, empirical screening level models were developed to correlate phosphorus loads to lakes with the resulting ambient levels of phosphorus and algal biomass as chlorophyll (e.g., Dillon and Rigler, 1974). Some screening models have also been developed that represent the partitioning of the total phosphorus input as: inorganic phosphorus; detrital particulate organic phosphorus; and living algal biomass as the stoichiometric equivalent of phosphorus (Schnoor and O'Connor, 1980). The mass of conventional pollutants available in the sediment bed is not represented in this type of a simple model. Screening level models of conventional pollutants and eutrophication are too simplified to be technically acceptable for the purposes of this study.

Intermediate level models of conventional pollutants and eutrophication are designed to represent the time-variable pathways and interactions of carbon, nitrogen, phosphorus and dissolved oxygen in a simplified aquatic food web consisting of a single, lumped species group of water column algae. In an intermediate model, algae in the water column are explicitly coupled with the supply of nutrients and the photosynthetic source and respiratory losses of dissolved oxygen. In an intermediate model, the pools of total organic carbon and total organic nutrients are simplified by combining the (a) dissolved and particulate forms; and (b) labile (fast reacting) and refractory (slow reacting) forms of these constituents. In some intermediate models, organic carbon is represented as the oxygen equivalent form as CBOD. Intermediate models typically represent chlorophyll dependent light extinction in the water column. The representation of light extinction resulting from the optical properties of water, including color, and the quantity of suspended inorganic and detrital organic matter is parameterized in intermediate models by specification of light extinction due to "non-algae" processes. Intermediate level models can represent coupling of carbon, nutrients and oxygen between the water column and the sediment bed with fluxes of nutrients and dissolved oxygen across the sediment-water interface provided either as (a) external user supplied input data or (b) internal results computed by a simplified benthic flux sub-model of organic carbon decay in the sediment bed. Intermediate level models for conventional pollutants and eutrophication generally allow for eight to twelve state variables to describe simplified biogeochemical processes and interactions.

The most complex, or advanced, conventional pollutant and eutrophication models account for detailed descriptions of the interrelated processes involving nutrients, suspended solids, dissolved oxygen and algae. In contrast to the simpler, intermediate level models, an advanced water quality eutrophication model represents organic carbon and organic nutrients as dissolved, particulate, labile and refractory forms. An advanced eutrophication model allows for the representation of multiple species of algae to describe seasonal succession in the water column. The most advanced eutrophication models also represent benthic algae and macrophytes as primary producer components of shallow aquatic ecosystems. Light extinction in the water column in an advanced model is internally coupled with algal biomass and suspended solids to provide a complete description of all the processes that govern light adsoprtion in the water column. Finally, advanced water quality and eutrophication models are designed to explicitly link changes in external loading of nutrients, suspended solids and organic carbon and the deposition of particulate organic carbon with sediment diagenesis and the resulting flux of nutrients and dissolved oxygen across the sediment-water interface. Complex conventional pollutant and eutrophication models typically have from 20 to 24 water quality state variables and incorporate a state-of-the-art sediment diagenesis model to explicitly couple organic matter produced in the water column with biogeochemical processes in the sediment bed.

In reviewing and evaluating the various features or processes of a conventional pollutant transport and fate model, the detailed assessment of candidate models focused on (*a*) the capability of a candidate model to represent a key feature, attribute, process or interaction; and (*b*) the level of detail of the formulation(s) used to describe the processes or interactions. When the model comparisons are used for selection of a model, the 'conceptual model' of the site-specific problem setting will determine which attributes of the head-to-head comparison are the most relevant.

As a component of a broader contaminated sediment modeling system, the critical function of the conventional pollutant transport and fate model is to represent the creation and decomposition of particulate organic matter, or organic sediment via eutrophication modeling. The evolution of eutrophication modeling schemes has been driven by the ability/inability of existing models to adequately represent the processes that dominate nutrient cycling in critical environmental settings or conditions. Generally speaking, model inadequacies are identified, and models are enhanced, when the model(s) cannot re-create the observed timing and amount of cycling between measured state variables. The earlier and simpler eutrophication models have been progressively enhanced to include better representation of phenomena such as the following:

- <u>Residence time of organic materials</u>. The need has been recognized to differentiate between particulate forms that may settle out of the water column and dissolved forms that remain in the water column unless they are transformed.
- <u>Decomposition of organic materials</u>. The need has been recognized to differentiate between multiple categories of organics that decompose at significantly different rates.
- <u>Availability of inorganic nutrients</u>. The need has been recognized to more fully represent processes that affect the immediate availability of dissolved nutrients for uptake by biota. For example, in numerous cases it has proven necessary to represent (1) the adsorption of nutrients to organic or inorganic sediment with subsequent sediment-driven transport and (2) the production of nutrients via diagenesis in bed sediments and their subsequent release into the water column.
- <u>Algal species succession</u>. In receiving waters that are characterized by significant populations of multiple algal species (blue-green, green, diatoms) and macrophytes, the amount or timing of nutrient cycling cannot be represented without enabling modelers to characterize multiple species with different temperature and feeding preferences.
- <u>Impacts of higher trophic levels (i.e., invertebrates, fish) on nutrient cycling</u>. The need for representing an expanded set of biotic state variables and processes has been recognized, and is driving current interest in enhancing eutrophication models to include ecologically-based algorithms.

*<u>Comparison C1: Tracking Scheme for Dead Reacting Organic Materials.</u>* There are three state variable schemes for tracking dead reacting organic materials: track as *biochemical oxygen demand*, track as *organic matter*, or track as *organic carbon.*

*<u>Comparison C2: Detail in Tracking Dead Reacting Organic Materials.</u>* Materials include CBOD (if modeled), reacting organic P, N and/or C (if modeled). Models either (1) lump particulate and dissolved forms and apply a single settling rate to the lumped quantity or (2) model particulate and dissolved forms separately.

*<u>Comparison C3: Detail in Representing Decomposition.</u>* To represent decomposition, models either use (1) one pool of decaying materials with one reaction rate or (2) multiple pools of decaying materials, each with its own decay rates.

*<u>Comparison C4: Reactivity of Organic Nitrogen and Phosphorus.</u>* There are three different schemes used to model reactivity of organic N and P. In some models organic N and P are not modeled at all; in other models the two state variables are modeled, but are non-reactive; still other models represent decay of organic N and P via mineralization and/or hydroloysis.

*<u>Comparison C5: Sediment-Ammonia Interaction.</u>* There are four approaches used for representing sediment-ammonia interaction in the water column: (1) represent adsorption-desorption of ammonia to inorganic sediment, (2) represent 'effective' adsorption-desorption of ammonia to inorganic sediment, (3) represent irreversible adsorption and loss to sediment, or (4) no representation of adsorption-desorption.

*<u>Comparison C6: Sediment-Phosphate Interaction.</u>* There are four approaches used for representing sediment-phosphate interaction in the water column: (1) represent adsorption-desorption of phosphate to inorganic sediment, (2) represent 'effective' adsorption-desorption of phosphate to inorganic sediment, (3) represent irreversible adsorption and loss to sediment, or (4) no representation of adsorption-desorption.

<u>Comparison C7: Sediment Oxygen Demand.</u> Models use either *descriptive* or *mechanistic* sediment oxygen demand and benthal releases of CBOD and dissolved nutrients. Descriptive demands and releases are represented using zero order kinetics. Mechanistic demands and releases are represented using first order kinetics.

*<u>Comparison C8: Sediment Diagenesis.</u>* Models may or may not represent sediment diagenesis, i.e. the coupled simulation of state variable interactions in the water column and the bed sediment to predict SOD and benthal nutrient releases.

*<u>Comparison C9: Plankton.</u>* Models use different plankton schemes: (1) represent one compartment each for floating algae, benthic algae & zooplankton, (2) represent one compartment for floating algae, or (3) represent multiple compartments for floating algae.

The conventional pollutant transport and fate models selected for review and evaluation include the following models:

AQUATOX V2.0
EFDC and EFDC1D
CE-QUAL-ICM V1.0

HSPF-RCHRES V12.0
WASP5-EUTRO5 V5.10 and WASP6-EUTRO6 V6.1

Table 3.4 presents a comparison of the state variables represented in each model. Table 3.5 presents a comparison of the kinetic processes and interactions incorporated in each model.

Intermediate Models. HSPF-RCHRES, WASP5-EUTRO5 and WASP6-EUTRO6 are all considered intermediate level conventional pollutant transport and fate models. These models are classified as intermediate level models for the following reasons: (1) primary producer species groups are lumped as single species groups of algae, benthic algae and/or macrophytes in a simplified aquatic food chain representation; (2) biogeochemical reactions for total organic nutrients (N and P) and total organic carbon combine the dissolved/particulate components and labile/refractory components as lumped state variables; (3) internal processes that influence biological production and the abundance of algal biomass, such as light extinction in the water column and zooplankton predation, are represented by parameterized and/or empirical relationships provided as input data to the models; and (4) mass fluxes of nutrients and dissolved oxygen (sediment oxygen demand) across the sediment-water interface are represented by empirical, external forcing functions provided as input data to the models.

WASP5-EUTRO5 and WASP6-EUTRO6 represent primary producers as a single lumped class of water column algae. Benthic algae and/or macrophytes are not available as state variables in these WASP “cousins”. HSPF-RCHRES represents primary producers as a single lumped class of water column algae as well as multiple groups of benthic algae and/or macrophytes as state variables. In both HSPF-RCHRES and WASP5-EUTRO5 and WASP6-EUTRO6, primary producer growth rates and productivity are simulated as non-linear relationships dependent on water temperature, the availability of light and the availability of inorganic nitrogen and phosphorus. Silica is not considered as a nutrient required for diatoms in these intermediate models since algae are represented only as a lumped assemblage of phytoplankton. In these intermediate models, algal biomass is allowed to settle out of the water column to the bed via a user-assigned settling velocity. Deposition and resuspension processes that affect detrital organic matter as well as algal biomass are not included in the intermediate class of models as physical processes that control the vertical transport of algal biomass between the water column and the bed. HSPF-RCHRES is the only intermediate model designed to represent herbivorous zooplankton as a dynamic state variable in the simplified aquatic food chain. The WASP5-EUTRO5 and WASP6-EUTRO6 models account for the loss of algal biomass by zooplankton grazing as an external forcing function for zooplankton biomass and/or a parameterized zooplankton grazing rate to estimate mortality from predation. None of the intermediate models include trophic levels any higher than herbivorous zooplankton in their representation of the aquatic food chain.

The intermediate models represent the inorganic forms of nitrogen and phosphorus and the organic forms of nitrogen, phosphorus and carbon. Organic carbon is represented in these models as carbonaceous biochemical oxygen demand (CBOD) where CBOD is the oxygen-equivalent of total organic carbon ($O_2$:C = 2.67 g $O_2$/g C). The organic nutrients and carbon state variables represent total organic nitrogen, total organic phosphorus and total organic carbon as CBOD. The dissolved and particulate forms of the nutrients and organic carbon (as CBOD) are only indirectly represented using forcing functions based on the user’s input of empirically determined dissolved fractions of organic matter. Labile and refractory differences in the reaction rates for decay are not considered in these intermediate models. The decay rates

| 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.

**Table 3.4 Comparison of Conventional Pollutant Transport and Fate Model State Variables (concluded)**

| | AQUATOX V.2.0 | CE-QUAL-ICM V.1 | EFDC | HSPF-RCHRES V.12 | WASP5(6)-EUTRO5(6) |
|---|---|---|---|---|---|
| **Silica** | | | | | |
| Available Silica | ★ | ★ | ★ | | |
| Particulate Biogenic Silica | | ★ | ★ | | |
| **Organic Matter/Detritus[1]** | | | | | |
| Total Organic Matter (Dissolved + Particulate) | | | | ★ | ★ |
| Particulate Organic Matter (Labile + Refractory) | | | | | |
| Particulate Organic Matter (Labile) | ★ | ★ | ★ | | |
| Particulate Organic Matter (Refractory) | ★ | ★ | ★ | | |
| Dissolved Organic Matter (Labile + Refractory) | | ★ | ★ | | |
| Dissolved Organic Matter (Labile) | ★ | | | | |
| Dissolved Organic Matter (Refractory) | ★ | | | | |
| Buried Particulate Organic Matter (Labile) | ★ | | | | |
| Buried Particulate Organic Matter (Refractory) | ★ | | | | |
| **Inorganic Carbon** | | | | | |
| Alkalinity | | | | ★ | |
| Total Inorganic Carbon | | | | ★ | |
| Carbon Dioxide | ★ | | | ★ | |
| pH | | | | | |
| **Other State Variables** | | | | | |
| Salinity/Chorides | | ★ | ★ | 2 | 3 |
| Total Suspended Solids | 4 | 4 | 4 | 2 | 5 |
| Total Active Metal | | ★ | ★ | | |

**footnotes**

**1** State variables for organic matter can be defined as: (a) carbonaceous biochemical oxygen demand; (b) organic carbon; or (c) dry w eight content. Organic matter can be represented as dissolved and particulate fractions and labile (fast reacting) and refractory (slow reacting) fractions. Dissolved organic matter is operationally defined as colloidal material w ith a particle size smaller than 0.45 micron. HSPF and WASP5(6)-EUTRO5(6) both simulate oxidizable organic matter as carbonaceous biochemical oxygen demand (CBOD). In WASP5(6)-EUTRO5(6), the dissolved and particulate fractions of oxidizeable organic matter (CBOD) are represented by user-defined dissolved fractions assigned as a spatially variable forcing function. In HSPF-RCHRES, an explicit representation of the dissolved and particulate fractions of organic matter (CBOD) is not considered. The particulate fraction of oxidizeable organic matter settles out of the w ater column via a user-defined settling velocity in both HSPF-RCHRES and WASP5(6)-EUTRO5(6). In CE-QUAL-ICM and EFDC, oxidizeable organic matter is simulated as organic carbon that is explicitly represented by dissolved and particulate fractions and labile and refractory components. In AQUATOX, organic matter is simulated as the dry w eight content of dissolved and particulate organic matter. Dissolved and particulate organic matter are also split into labile and refractory components. Equivalent concentrations of organic nitrogen, organic phosphorus and organic carbon are internally computed using stoichiometric ratios of carbon:dry w eight (C:DW); carbon:nitrogen (C:N) and nitrogen:phosphorus (N:P) for detritus.

**2** Modeled as a generalized conservative substance

**3** Salinity/chlorides is a state variable in WASP 6.1; in WASP5-EUTRO5 salinity is not a state variable, but it is input as an external space- and time-varying forcing function.

**4** In AQUATOX TSS is computed as the sum of sands + silts + clays + detrital POM + algal biomass POM. In

**Table 3.5 Comparison of Conventional Pollutant Transport and Fate Model Processes**

| | AQUATOX V2.0 | CE-QUAL-ICM V.1 | EFDC | HSPF-RCHRES V.12 | WASP5(6)-EUTRO5(6) |
|---|---|---|---|---|---|
| **Water Column Algae/Primary Producers** | | | | | |
| Photosynthetic Growth as Function of Light, Temperature and Nutrients | 2 | 2 | 2 | ★ | ★ |
| Respiration as Function of Temperature | 2 | 2 | 2 | ★ | ★ |
| Mortality Due to Environmental Stresses | 2 | 2 | 2 | ★ | ★ |
| Mortality Due to Chemical Toxicity | 2 | | | | |
| Mortality Due to Zooplankton Predation | ★ | 3 | 3 | ★ | 4 |
| Mortality Due to Higher Trophic Level Predation | ★ | | | | |
| Nitrogen Fixation by Blue-Green Algae | ★ | | | | |
| Settling of Biomass Assigned as Input to Model | ★ | ★ | ★ | ★ | ★ |
| Deposition and Resuspension of Biomass Computed as Function of Bottom Stress | 7 | | | | |
| **Benthic Algae/Primary Producers** | | | | | |
| Photosynthetic Growth as Function of Light, Temperature and Nutrients | ★ | | ★ | 5 | |
| Respiration as Function of Temperature | ★ | | ★ | 5 | |
| Sloughing of Attached Biomass from Bottom | ★ | | ★ | 5 | |
| Resuspension of Biomass Computed as Function of Bottom Stress | ★ | | | | |
| **Macrophytes** | | | | | |
| Growth, Respiration and Death | ★ | | | 6 | |
| Excretion and Predation | ★ | | | | |
| **Zooplankton** | | | | | |
| Grazing & Predation as Function of Prey Biomass & Temperature | ★ | | | ★ | |
| Respiration as Function of Temperature | ★ | | | ★ | |
| Mortality by Predation | ★ | | | | |
| Non-predatory Mortality | ★ | | | ★ | |
| Excretion | ★ | | | ★ | |
| Egestion of Non-Assimilated Food | ★ | | | | |
| **Higher Trophic Levels** | | | | | |
| Feeding as Function of Food Source Biomass & Temperature | ★ | | | | |
| Respiration as Function of Temperature | ★ | | | | |
| Mortality by Predation | ★ | | | | |
| Non-predatory Mortality | ★ | | | | |
| Excretion | ★ | | | | |
| Egestion of Non-assimilated Food | ★ | | | | |
| **Pathogens** | | | | | |
| First-Order Decay as Function of Temperature | | | ★ | ★ | 8 |
| First-Order Decay as Function of Temperature, Light and Salinity/Chlorides | | | | | |
| Settling Velocity of Pathogens Sorbed to Sediment Assigned as Input | | | | | ★ |
| Deposition of Pathogens Sorbed to Solids Computed as Function of Bottom Stress | | | | 1 | |
| Resuspension of Pathogens Sorbed to Solids Computed as Function of Bottom Stress | | | | 1 | |

**footnotes**

**1** Since pathogens are simulated as a generalized constituent in HSPF, representation of sorption to inorganic sediment and subsequent deposition and resusupension is possible.

**2** Represents processes for three groups of algae (green, diatoms, cyanobacteria) independently.

**3** Zooplankton are not modeled as a state variable; rather, effect of zooplankton is simulated assuming constant relationship between algal mass and zooplankton mass. The loss of algae is first order w.r.t. algal mass.

**4** Zooplankton are not modeled as a state variable; rather, the effect of zooplankton is simulated by a user input time dependent zooplankton population grazing at a user specified rate, or by assuming a constant relationship between algal mass and zooplankton mass. The loss of algae is first order w.r.t. algal mass.

**5** Multiple benthic algae comparments are allowed in HSPF.

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

**7** Deposition is constrained by discharge and wind.

**8** Process represented in WASP(6), but not WASP(5).

**Table 3.5. Comparison of Conventional Pollutant Transport and Fate Model Processes (continued)**

| | AQUATOX V2.0 | CE-QUAL-ICM V.1 | EFDC | HSPF-RCHRES V.12 | WASP5(6)-EUTRO5(6) |
|---|---|---|---|---|---|
| **Nutrient Biogeochemical Processes and Interactions in Water Column** | | | | | |
| Inorganic Phosphorus (Phosphate) Adsorption/Desorption to Inorganic Suspended Sediment | | | | ★ | 2 |
| Ammonium Adsorption/Desorption to Inorganic Suspended Sediment | | | | ★ | 2 |
| Irreversible Adsorption of Phosphate to Sediment, Settling | | | | | |
| Ammonia Vaporization | | | | ★ | |
| Settling/Resuspension for Nutrients Adsorbed to Sediment | | | | ★ | |
| Settling Velocity of Particulate Nutrients Assigned as Input to Model | ★ | ★ | ★ | ★ | ★ |
| Deposition of Particulate Nutrients Computed as Function of Bottom Stress | | | | | |
| Resuspension of Particulate Nutrients Computed as Function of Bottom Stress | | | | | |
| Phosphate Exchange with Particulate Metals | | ★ | ★ | | |
| Mineralization of Detrital Organic Nutrients (Dissolved + Particulate) | ★ | | | ★ | ★ |
| Hydrolysis/Dissolution of Detrital Organic Nutrients to Dissolved Organic Nutrients | ★ | ★ | ★ | | |
| Mineralization of Dissolved Organic Nutrients to Inorganic Nutrients | ★ | ★ | ★ | | |
| Nitrification | ★ | ★ | ★ | ★ | ★ |
| Denitrification | ★ | ★ | ★ | ★ | ★ |
| **Nutrient Interactions with Primary Producers** | | | | | |
| Nutrient Uptake by Water Column Algae | ★ | ★ | ★ | ★ | ★ |
| Nutrient Uptake by Benthic Algae | ★ | | ★ | ★ | |
| Nutrient Uptake by Macrophytes | ★ | | | 1 | |
| Nutrient Release by Algal Respiration/Death/Decomposition | ★ | ★ | ★ | ★ | ★ |
| Nutrient Release by Benthic Algae Respiration/Death/Sloughing/Decomposition | ★ | | ★ | ★ | |
| Nutrient Release by Macrophyte Respiration/Death/Decomposition | ★ | | ★ | 1 | |
| **Nutrient Interactions with Grazers & Predators** | | | | | |
| Nutrient Release by Zooplankton Respiration/Mortality/Excretion/Egestion | 3 | | | ★ | |
| Nutrient Release by Higher Trophic Level Respiration/Mortality/Excretion/Egestion | ★ | | | | |
| **Nutrient Biogeochemical Processes and Interactions in Sediment Bed** | | | | | |
| Sediment Bed Release of Ammonia (NH4) & Phosphate (O-PO4) Assigned as Input to Model | ★ | | | 4 | ★ |
| Sediment Bed Release of Nitrate + Nitrite (NO3+NO2) Assigned as Input to Model | ★ | | | | |
| Sediment Bed Release of Available Silica Assigned as Input to Model | | | | | |
| Sediment Bed Nutrient Concentration Computed from Sediment Diagenesis Model | | ★ | ★ | | |
| Sediment Bed Release of Nutrients Computed from Simplified Bed Decomposition Model | ★ | | | | ★ |
| Sediment Bed Nitrification | ★ | ★ | ★ | | ★ |
| Sediment Bed Denitrification | ★ | ★ | ★ | | ★ |
| **Dissolved Oxygen** | | | | | |
| Oxidation of Detrital Organic Matter | ★ | ★ | ★ | ★ | ★ |
| Nitrification | ★ | ★ | ★ | ★ | ★ |
| Phytoplankton Photosynthesis and Respiration | ★ | ★ | ★ | ★ | ★ |
| Benthic Algae Photosynthesis and Respiration | ★ | ★ | ★ | ★ | |
| Macrophyte Photosynthesis and Respiration | ★ | ★ | ★ | 1 | |
| Heterotrophic Respiration of Dissolved Organic Carbon | ★ | ★ | ★ | | |
| Zooplankton Respiration | ★ | | | ★ | |
| Higher Trophic Levels Respiration | ★ | | | | |
| Atmospheric Reaeration | ★ | ★ | ★ | ★ | ★ |
| Chemical Oxygen Demand Oxidation | | ★ | ★ | | |
| Sediment Oxygen Demand Assigned as Input to Model | | | | ★ | ★ |
| Sediment Oxygen Demand Computed from Simplified Bed Decomposition Model | ★ | | | | ★ |
| Sediment Oxygen Demand Computed from Sediment Diagenesis Model | | ★ | ★ | | |

**footnotes**

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

**2** Although there are no sediments modeled as state variables, this process is modeled by specifying fractions of phosphate which are particulate. As dissolved nutrients are depleted, the model reduces the quantity of

**Table 3.5. Comparison of Conventional Pollutant Transport and Fate Model Processes (concluded)**

| | AQUATOX V.2.0 | CE-QUAL-ICM V.1 | EFDC | HSPF-RCHRES V.12 | WASP5(6)-EUTRO5(6) |
|---|---|---|---|---|---|
| **Carbonaceous Biochemical Oxygen Demand (CBOD)** | | | | | |
| Algal Death/Decomposition/Excretion | | | | ★ | ★ |
| Benthic Algae Death/Decomposition/Excretion | | | | ★ | |
| Macrophyte Death/Decomposition | | | | 1 | |
| Zooplankton Death and Excretion | | | | ★ | |
| Zooplankton Predation | | | | ★ | 4 |
| Oxidation of Detrital Organic Matter | | | | ★ | ★ |
| Hydrolysis of Detrital Organic Matter | | | | | |
| Heterotrophic Respiration | | | | | |
| Denitrification | | | | | ★ |
| Settling Velocity of Particulate Organic Matter Assigned as Input | | | | ★ | ★ |
| Sediment Release of CBOD to Water Column Assigned as Input to Model | | | | 6 | |
| Deposition of Particulate Fraction of CBOD Computed as Function of Bottom Stress | | | | | |
| Resuspension of Particulate Fraction of CBOD Computed as Function of Bottom Stress | | | | | |
| **Organic Carbon (DOC & POC)/Detrital Organic Matter (DOM & POM)** | | | | | |
| Algal Death/Decomposition/Excretion | 2 | 2 | 2 | | |
| Benthic Algae Death/Decomposition/Excretion | ★ | ★ | ★ | | |
| Macrophyte Death/Decomposition | ★ | | | | |
| Zooplankton Death/Excretion | 3 | | | | |
| Zooplankton Predation | 3 | 5 | 5 | | |
| Oxidation of Detrital Organic Matter | ★ | ★ | ★ | | |
| Hydrolysis of Detrital Organic Particulate Matter | ★ | ★ | ★ | | |
| Heterotrophic Respiration of Dissolved Organic Carbon | ★ | ★ | ★ | | |
| Denitrification | ★ | ★ | ★ | | |
| Settling Velocity of Particulate Organic Matter Assigned as Input | ★ | ★ | ★ | | |
| Deposition of Particulate Organic Matter Computed as Function of Bottom Stress | 7 | | | | |
| Resuspension of Particulate Organic Matter Computed as Function of Bottom Stress | | | | | |
| Dissolution of Particulate Organic Matter to Dissolved Organic Matter | ★ | ★ | ★ | | |
| Sediment Bed Organic Carbon Concentration Computed from Sediment Diagenesis Model | | ★ | ★ | | |
| **Inorganic Carbon & pH** | | | | | |
| Atmospheric Exchange | ★ | | | ★ | |
| Primary Producer Photosynthesis and Respiration | ★ | | | ★ | |
| Zooplankton Respiration | 3 | | | ★ | |
| Sediment Release of $CO_2$ to Water Column Assigned as Input to Model | | | | ★ | |
| Decomposition of Detrital Organic Matter | ★ | | | | |

**footnotes**

**1** One of multiple benthic algae compartments can be used to model macrophytes.
**2** Represents processes for three groups of algae (green, diatoms, cyanobacteria) independently.
**3** Represents processes for multiple zooplankton groups
**4** Zooplankton are not modeled as a state variable; rather, effect of zooplankton is represented by a user input time dependent zooplankton concentration and a user input algae predation rate. This process serves only to reduce algal concentration.
**5** Zooplankton are not modeled as a state variable; rather, effect of zooplankton is simulated assuming constant relationship betw een algal mass and zooplankton mass.
**6** Step increases in release rate are triggered by low DO or high velocity conditions.
**7** Deposition is constrained by discharge and w ind.

represent the composite effect of both slow (refractory) and fast (labile) reacting fractions of organic nutrients and organic carbon. Of the intermediate models, HSPF-RCHRES is the only model that includes a mass balance of inorganic carbon to simulate alkalinity and carbon dioxide.

Salinity and/or chlorides are represented as a state variable only in WASP6-EUTRO6. In WASP5-EUTRO5, salinity and/or chlorides is described by space/time forcing functions that are provided as input data to the model. In HSPF-RCHRES, salinity and/or chlorides can be modeled as a generalized conservative substance.

Total suspended solids, including organics, are not explicitly considered in either HSPF-RCHRES or the WASP-EUTRO "cousins". HSPF-RCHRES simulates inorganic solids (clays, silts, sands) and CBOD. Since the dissolved fraction of CBOD is not defined in HSPF-RCHRES, the equivalent particulate organic carbon and particulate organic matter (as dry weight) concentrations cannot be determined. It is thus not possible to compute total suspended solids (inclusive of the organic fraction) as an output variable from HSPF-RCHRES. Three classes of suspended solids are available as state variables in the WASP5-TOXI5 and WASP6-TOXI6 toxics models. However, suspended solids are not available as a state variable in the eutrophication version of the WASP "cousins". The effect of suspended solids on light extinction in the water column is parameterized in WASP5-EUTRO5 and WASP6-EUTRO6 using an empirically determined external forcing function that assigns light extinction related to non-algal particulate matter and water color as input to the model. The effect of algal biomass on light extinction is internally computed using a functional relationship developed by Riley (1956) with the simulated algal biomass concentration. The incremental effects on light extinction of algae concentration and total suspended inorganic sediment concentration are represented empirically in HSPF-RCHRES.

HSPF-RCHRES can account for pathogens, such as fecal coliform bacteria, using a state variable designed as a generalized water temperature-dependent reactive constituent. This is a simplification of the environmental factors that influence the mortality of coliform bacteria since bacterial mortality is dependent on the availability of light and the fraction of seawater as salinity and/or chlorides (Mancini, 1978 and Chapra, 1997). WASP5-EUTRO5 does not represent pathogens as a state variable. The more recently released Version 6.1 of WASP (Wool et al., undated) includes a new WASP model framework that includes fecal coliform bacteria and water temperature as state variables. A modified version of WASP5-EUTRO5, developed by Research Triangle Institute (RTI) for EPA's National Water Pollution Control Assessment Model (NWPCAM, Version 2.0) (Bondelid et al., 2002), incorporates inorganic suspended solids, salinity/chlorides and coliform bacteria as additional state variables for the water quality/eutrophication model.

The kinetic reactions that influence dissolved oxygen are essentially identical in HSPF-RCHRES and the WASP "cousins". Kinetic terms in the oxygen sub-model include: production of oxygen from primary producer photosynthesis; uptake of oxygen from primary producer respiration; loss of oxygen via nitrification and decomposition of organic matter; the transfer of oxygen from the atmosphere to the water column via reaeration; and the loss of oxygen across the sediment-water interface via decomposition of organic matter in the sediment bed (i.e., sediment oxygen demand or SOD).

HSPF-RCHRES, WASP5-EUTRO5 and WASP6-EUTRO6 account for the mass flux of inorganic nutrients and dissolved oxygen across the sediment-water interface as externally defined, empirical space/time forcing functions provided as input data to these models. Sediment oxygen demand (SOD) rates are assigned on the basis of either site-specific field measurements or best estimates based on the technical literature. Benthic nutrient flux rates for ammonia-N, ortho-phosphate-P and nitrate-N + nitrite-N are assigned on the basis of either site-specific field measurements or as stoichiometric equivalents computed from the assigned SOD rates and the 'Redfield' ratios of C:N, C:P, and O2:C (Redfield et al., 1963; Di Toro, 2000). In addition to the empirical method based on the assigned input of SOD and benthic nutrient flux rates, WASP5-EUTRO5 and WASP6-EUTRO6 also provide the option to activate a simplified sub-model that couples particulate organic matter deposition to the sediment bed with an internal simulation of SOD and benthic nutrient regeneration rates. This simplified model, originally developed for an analysis of anoxia in Lake Erie (Di Toro and Connolly, 1980), was applied to the Potomac estuary (Thomann and Fitzpatrick, 1982) and incorporated in Version 4 of the WASP eutrophication model (Ambrose et al., 1988). In subsequent work on the problem of sediment bed decomposition, Di Toro et al. (1990) and Di Toro (2000) developed an elegant model of sediment diagenesis that is now incorporated in advanced water quality eutrophication models such as RCA, CE-QUAL-ICM and EFDC.

Advanced Models. AQUATOX, EFDC and EFDC1D, and CE-QUAL-ICM are considered advanced conventional pollutant transport and fate models. These models are classified as advanced models for the following reasons: (1) primary producer species groups are split as multiple species groups of algae (e.g., diatoms, blue-greens, greens dinoflagellates etc), benthic algae and macrophytes in a complex aquatic food chain representation; (2) biogeochemical reactions for organic nutrients and organic carbon are split into dissolved/particulate components with the dissolved/particulate components further split as labile and refractory components as separate state variables; (3) internal processes that influence biological production and the abundance of algal biomass, such as light extinction in the water column and zooplankton predation, are represented by functional relationships coupled with internally simulated suspended solids and zooplankton abundance; and (4) mass fluxes of nutrients and dissolved oxygen across the sediment-water interface are simulated using a state-of-the-art sediment diagenesis model that is internally coupled with the deposition of particulate organic carbon to the sediment bed (Di Toro et al., 1990; Di Toro, 2000).

AQUATOX, CE-QUAL-ICM and EFDC and EFDC1D provide a detailed representation of primary producers in natural waters. Functional groups of algae represented in these models include: diatoms, blue-greens, greens, and dinoflagellates. Benthic algae are incorporated in AQUATOX, CE-QUAL-ICM and EFDC and EFDC1D. Macrophytes are explicitly represented only in AQUATOX. In all of these advanced models, primary producer growth rates and productivity are simulated as non-linear relationships dependent on water temperature, the availability of light and the availability of inorganic nitrogen and phosphorus. Silica, required for diatom growth, is included as an additional inorganic nutrient in these advanced models. In both the advanced and intermediate models, algal biomass for each functional group is allowed to settle out of the water column to the bed via user-assigned settling velocities. Deposition and resuspension processes that affect detrital organic matter as well as algal biomass are not included in either the intermediate or advanced class of models as physical processes that determine the vertical transport of algal biomass between the water column and the bed. AQUATOX is the only advanced model designed to represent herbivorous zoooplankton as a dynamic state variable in a detailed aquatic food chain. Similar to the methods used in the

WASP-EUTRO models, CE-QUAL-ICM, EFDC and EFDC1D account for the loss of algal biomass by zooplankton grazing as an external forcing function for zooplankton biomass and/or a parameterized zooplankton grazing rate to account for algal mortality from predation. AQUATOX is the only advanced model that attempts to provide a realistic representation of the production, decomposition and transfers of organic matter and inorganic nutrients within an aquatic food web across all trophic levels in the water column (pelagic) and the sediment bed (benthic) compartments.

The advanced models represent the inorganic forms of nitrogen, phosphorus, silica and the organic forms of nitrogen, phosphorus and carbon. The organic nutrients and organic carbon state variables are split into dissolved/particulate forms with the dissolved and particulate components further split as labile/refractory components to account for differences in the reaction rates for decay. Decomposition thus accounts for the combined effects of slow (refractory) and fast (labile) reacting fractions of organic nutrients and organic carbon. Of the advanced models, AQUATOX is the only model that includes a mass balance of inorganic carbon to simulate carbon dioxide.

Salinity and/or chlorides are represented as state variables of the hydrodynamic models in CE-QUAL-ICM, EFDC and EFDC1D. Salinity and/or chlorides simulated in the hydrodynamic models are directly coupled with the water quality model. AQUATOX does not include salinity/chlorides as a state variable.

Multiple classes of generalized solids are represented as state variables in the sediment transport models of EFDC and EFDC1D. AQUATOX includes clays, silts and sands as inorganic solids state variables. The sediment transport model of AQUATOX has recently been verified against the sediment transport model of HSPF-RCHRES (Park, 2003). Solids deposition and resuspension velocities are provided to AQUATOX by linkage with an internal sediment transport model. Total suspended solids are computed as an output variable in these models as the sum of the multiple suspended solids classes, detrital organic matter and algal biomass (as dry weight). The effects of suspended solids and algal biomass on light extinction in the water column are included in these advanced models as functional relationships that are coupled with the internally simulated concentrations of suspended solids and algal biomass.

EFDC and EFDC1D are the only advanced models designed to account for pathogens, such as fecal coliform bacteria, as a state variable. Bacterial mortality is simulated as a simple temperature dependent function. The dependence of mortality on the availability of light and the fraction of seawater (as salinity/chlorides) (Mancini, 1978; Chapra, 1978) is not, however, considered in EFDC.

The kinetic reactions that influence dissolved oxygen are essentially identical in all the intermediate and advanced models. Kinetic terms for dissolved oxygen include: production of oxygen from primary producer photosynthesis; uptake of oxygen from primary producer respiration; loss of oxygen via nitrification and decomposition of organic matter; the transfer of oxygen from the atmosphere to the water column via reaeration; and the loss of oxygen across the sediment-water interface via decomposition of organic matter in the sediment bed (i.e., sediment oxygen demand or SOD). In contrast to the intermediate models, the advanced models also include a term to account for the loss of oxygen by heterotrophic respiration of DOC. Chemical oxygen demand is incorporated in CE-QUAL-ICM, EFDC and EFDC1D. AQUATOX includes the respiratory losses of oxygen from zooplankton and the pelagic and benthic organisms represented in all other trophic levels.

AQUATOX accounts for the mass flux of inorganic nutrients and dissolved oxygen across the sediment-water interface by coupling the deposition of particulate organic matter to the bed with a simplified model of organic matter decomposition in the sediment bed. CE-QUAL-ICM, EFDC and EFDC1D simulate the mass fluxes of inorganic nutrients and dissolved oxygen (sediment oxygen demand or SOD) across the sediment-water interface using a state-of-the-art sediment diagenesis model that is internally coupled with the deposition of particulate organic carbon to the sediment bed (Di Toro et al., 1990; Di Toro, 2000). Over the past decade, the availability of a sediment diagenesis model has enabled modelers to accurately simulate the biogeochemical effect of implementing remediation plans designed to reduce nutrients and organic carbon loads on reductions in sediment oxygen demand rates and corresponding improvements in dissolved oxygen levels over decadal time scales. CE-QUAL-ICM and EFDC, for example, have been used to simulate decadal time scale reductions in sediment oxygen demand, benthic nutrient regeneration rates and improvements in near-bottom dissolved oxygen levels for Chesapeake Bay (Cerco and Cole, 1993) and Peconic Bay (Tetra Tech, 1999c).

### 3.2.4 Hydrodynamic Models

The water in streams, rivers, lakes, reservoirs, tidal rivers, estuaries and the oceans is in constant motion at all time scales. Water flows swiftly in clear, cold mountain streams. Water flows slowly in meandering rivers. Water can appear to be motionless in a lowland swamp. The motion of water in tidal rivers and estuaries is controlled by freshwater inflow from rivers at the upstream end of the waterway, the influx of salt from the ocean and the daily fluctuation of the tides at the downstream connection with the ocean. Fluid flow in the open ocean is driven by the tides, winds, water density, and the rotation of the earth while water flow in the coastal ocean is also governed by freshwater inflow from rivers discharging into the sea and the geometries of the coastline and the bottom depth of the continental shelf. These and other physical factors that govern the motion of water in bodies of water open to the atmosphere at the air-sea interface have been identified and studied for many years by scientists, engineers and mathematicians in the disciplines of open channel hydraulics, physical oceanography, limnology and fluid mechanics.

<u>Equations of Fluid Motion</u>

Newton's second law of motion defines the acceleration of a fluid in terms of mass and the change of velocity of the fluid with time. First defined in the mid-nineteenth century, a complete description of the physical factors that govern surface water motion were written as the 'Navier-Stokes' equations of motion. These equations of fluid motion contain a number of terms that describe the time-dependency of the acceleration of a fluid in three dimensions. The equations of fluid motion are based on the fundamental principles of conservation of momentum, mass and energy. Measurable extrinsic properties like water temperature, concentration of salt and other constituents, flow, and velocity are used as the state variables of a model to generate solutions of water surface elevation and velocity.

Partial derivative terms for velocity and pressure are included in the 'Navier-Stokes' equations that define the non-linear advection of momentum, spatial gradients of pressure, frictional effects, the rotation of the earth, and gravitational acceleration. Pressure gradient terms, expressing the commonly known principles that heavy water sinks and water flows downhill, define the influence of spatial differences in water density and elevation of the water surface. Friction terms describe the stress effects of wind forcing at the air-water interface, internal turbulent motion and the effect of bottom drag at the sediment-water interface. In order to apply the equations of motion to descriptions of the circulation of water in the ocean or large lakes and bays, the effect of the rotation of the earth is added as an artificial non-physical 'Coriolis force' to account for the relative motion of a parcel of water in the ocean with respect to a rotating coordinate system. The Coriolis 'force' defines the effect of the earth's rotation on the apparent motion of water in the open ocean.

Walsh (1988) provides a clear description of the mathematical terms incorporated in the 'Navier-Stokes' equations and the approximations that have been made to generate analytical and numerical model solutions. Cheng and Smith (1990) and Sheng (1990) both provide good overviews of the various approximations employed in modern three-dimensional hydrodynamic models. Martin and McCutcheon (1999) provide in-depth descriptions of the equations of motion and how those equations have been used to develop hydraulic models and hydrodynamic models. Most relevant to the reader of this document, Walsh (1988), Martin and McCutcheon (1999) and Lung (2001) present descriptions of hydrodynamics, not from the viewpoint of a physical oceanographer or applied mathematician, but from the perspective that hydrodynamic models are an integral component of a comprehensive framework for the development of water quality, eutrophication, sediment transport, toxic chemical fate and transport and aquatic ecosystem models.

<u>Fundamental Principles of Fluid Flow Models</u>

Conservation of momentum, mass and energy provide the fundamental principles needed to develop models of fluid flow and mass transport in surface waters. In order to apply the complex conservation of momentum equations with conservation of mass and energy equations, many simplifying assumptions are made to carefully delete, or scale, the numerous forces in the equations to arrive at tractable, yet meaningful, solutions that can provide scientific insight for a specific problem setting. Fluid flow models based on these principles are classified as either (a) hydraulic or (b) hydrodynamic models.

<u>Hydraulic models</u>, developed only for one-dimensional applications for lateral and depth averaged streams, rivers and tidal rivers, generally require a number of simplifying approximations to the equations of motion. In some cases, hydraulic models have evolved from empirical approximations such as the well known Manning's equation for steady state open channel flow calculations. Even this simplified approximation is based on conservation of momentum and the elimination of acceleration terms in the equations of motion except for the balance of forces governed by the bottom slope and bottom friction.

<u>Hydrodynamic models</u>, in contrast to the much simpler hydraulic models, use fewer approximations to the equations of fluid motion to increase physical realism. Using the 'Navier-Stokes' equations for fluid motion, hydrodynamic models account for the transport and mixing of surface water where water motion in the horizontal (x,y) and vertical dimensions (z) is influenced by cross-sectional area, depth and bottom slope of the water body, freshwater inflows, water surface elevation and physical processes such as bottom friction, winds, turbulent mixing and vertical stratification induced by water temperature and salt content (i.e., density). In estuarine and coastal waters the distributions of salt and tidal forcing are major factors that control circulation processes.

Hydrodynamic models, constructed to represent realistic geometry of shorelines and bathymetry with two-dimensional and three-dimensional grids, require advanced numerical methods to solve the time dependent equations for the distributions of water surface elevation, salt, water temperature and velocity.

Evolution of Fluid Flow Models

The large number of computer models developed to solve the equations of fluid motion, now available to practicing engineers and scientists, have evolved over the past 30 years largely in response to three key factors: (1) mathematical necessity to apply approximations to the equations of motion to describe the transport of water in rivers, lakes, estuaries and oceans; (2) availability of computer technology; and (3) availability of numerical methods to perform the necessary calculations. The increasing availability of very powerful, affordable and widely accessible computer technology in combination with the availability of advanced numerical methods has enabled the development of physically realistic models designed to simulate water movement in complex surface water systems. These advanced models contain very few simplifying approximations to the 'Navier-Stokes' governing equations of motion (see Cheng and Smith, 1990; Sheng, 1990).

Modern three-dimensional hydrodynamic models, which can also be readily applied for one- and two-dimensional problem settings, provide a powerful computational tool for advanced sediment transport, water quality, eutrophication and toxic chemical fate and transport modeling studies. The hydrodynamic model provides the (a) velocity and flow field, (b) elevation of the water surface, and (c) bottom stress. The velocity field and depth of the water column are used to determine mass transport of solids, toxicant and other constituents from advection and diffusion. Bottom stress is used to determine the exchange of a sorbed toxicant between the water column and sediment bed as a result of solids deposition and resuspension. Since the mid-1980s, advanced, three-dimensional hydrodynamic models (Blumberg and Mellor, 1987; Hamrick, 1992; Sheng, 1986) have successfully made the transition from academic research and development laboratories to practical applications of these models by environmental consulting firms, and state and federal agencies for water quality management studies of natural water systems. Modern hydrodynamic models have thus emerged as a critical component of environmental model frameworks for simulation studies of the transport of solids and toxic contaminants transport and fate in natural waters.

Waterbody Classifications and Spatial Dimensionality

One of EPA's minimum requirements for contaminated sediment models was that models selected for detailed analysis have "either an internal linkage or external coupling to a hydrodynamic model." As explained in Section 1.3, the Study Team determined that it was appropriate to consider, and characterize, hydrodynamic models as a component of this study. Within the context of this study, interest in hydrodynamic models is restricted to identifying the best models that are commonly used to drive the transport computations contained in the "best" sediment transport and chemical fate and transport models.

Consideration of hydrodynamic models stems from the study requirement that models usable for analysis of contaminated sediment problems in a broad range of water bodies be identified. With the exception of the hydrodynamic component, the computations contained in all other components (i.e., sediment transport, toxic chemical transport and fate, conventional pollutant transport and fate, eutrophication and sediment diagenesis) that are needed to implement a comprehensive contaminated sediment modeling system are "box models". These classes of models perform the same computations regardless of the type of site-specific water body. Hence, there is a need to identify, and compare, a select number of hydrodynamic models in order to differentiate between the best linked modeling systems for the spatial dimensionality of specific water body types.

Freshwater and saltwater/tidal water body types, presented in Table 3.6, are summarized below in relation to the dominance of one-, two- or three-dimensional (1D, 2D, 3D) spatial gradients of salt, water temperature and water quality constituents for the surface water system. Appendix B presents a more detailed discussion of the different types of waterbodies.

<u>One-Dimensional: 1D(x)</u>. A one-dimensional model is an appropriate representation for waterbodies in which the most significant water quality constituent gradient is along the longitudinal (x) axis in the direction of flow of the stream or river. The vertical (z) and lateral (y) dimensions are considered well-mixed since the gradient of a water quality constituent in these directions is considered to be negligible in relation to the dominant longitudinal (x) gradient. Free-flowing freshwater streams are shallow, high velocity, low-order waterbodies, typically characterized by steep hydraulic profiles with an alternating series of pools and riffles. Transport in a free-flowing stream is controlled by gravity in the absence of any influence from downstream obstructions. In a free-flowing stream, the application of a kinematic wave model, based on the St. Venant equations, is restricted to hydraulic conditions where the backwater effects from dams, or other obstructions to flow, are either negligible or non-existent. Transport in a higher-order freshwater river characterized by a moderate hydraulic profile, by contrast, is often controlled by the influence of downstream backwater effects induced by a dam, impoundment or blockage from debris. Tidal creeks and rivers, characterized by low salinity levels at the upstream (freshwater) end of the waterway, are typically narrow and shallow. Transport in a tidal waterway is controlled by upstream freshwater inflows and downstream fluctuations in surface water elevation that are controlled by tidal forcing.

<u>Two-Dimensional: 2D(x,y)</u>. A two-dimensional (horizontal), depth-averaged model is an appropriate representation for waterbodies where the most significant water quality constituent gradients are observed in the horizontal (x,y) dimensions. In a two-dimensional (horizontal) waterbody, the vertical dimension (z) is considered well-mixed since the vertical gradient of a water quality constituent is small in relation to the much larger horizontal gradients. Shallow/broad freshwater lakes and reservoirs or saltwater/tidal embayments and lagoons are typically represented with a 2D(x,y) model.

<u>Two-Dimensional: 2D(x,z)</u>. A two-dimensional (vertical), laterally-averaged model is an appropriate representation for waterbodies where the most significant water quality constituent gradients are observed in the longitudinal (x) and vertical (z) dimensions. Relatively deep, narrow stratified freshwater lakes, reservoirs, tidal rivers, estuaries and fjords are often modeled with a two-dimensional (vertical) representations. In a two-dimensional (vertical) stratified waterbody, the lateral dimension (y) is considered well-mixed since the lateral (or cross-shore) gradient of a water quality constituent is small in relation to the much larger vertical and longitudinal gradients.

**Table 3.6. Dimensional Requirements for Modeling Waterbody Types**

| | 1D(x) | 2D(xy) | 2D(xz) | 3D(xyz) |
|---|---|---|---|---|
| FRESHWATER SYSTEMS | | | | |
| Rivers & Streams: Free-Flowing and Backwater Effects | | | | |
| Vertically Well-mixed; Laterally Well-Mixed; Narrow & Shallow | ★ | | | |
| Vertically Well-Mixed; Lateral Gradients; Wide & Shallow | | ★ | | |
| Vertically Stratified; Laterally Well-Mixed; Narrow & Deep | | | ★ | |
| Vertically Stratified; Lateral Gradients; Wide & Deep | | | | ★ |
| Lakes/Bays & Reservoirs | | | | |
| Vertically Well-mixed; Lateral Gradients; Wide & Shallow | | ★ | | |
| Vertically Stratified; Laterally Well-Mixed; Narrow & Deep | | | ★ | |
| Vertically Stratified; Lateral Gradients; Wide & Deep | | | | ★ |
| SALTWATER/TIDAL SYSTEMS | | | | |
| Tidal Rivers & Embayments/Lagoons | | | | |
| Tidal Rivers: Vertically Well-Mixed; Laterally Well-Mixed; Narrow & Shallow | ★ | | | |
| Tidal Rivers: Vertically Well-Mixed; Lateral Gradients; Wide & Shallow | | ★ | | |
| Embayments/lagoons: Vertically Well-Mixed; Lateral Gradients; Wide & Shallow | | ★ | | |
| Estuaries & Coastal Ocean | | | | |
| Estuaries: Vertically Stratified; Laterally Well-Mixed; Narrow & Deep | | | ★ | |
| Estuaries: Vertically Stratified; Lateral Gradients; Wide & Deep | | | | ★ |
| Coastal Ocean: Vertically Stratified or Vertically Well-mixed; Narrow or Wide Shelf | | | | ★ |

**Table 3.7. Applicability of Hydrodynamic Models to Waterbody Types**

| | CH3D-WES V.1 | ECOM-3D V.1.3/POM | EFDC | EFDC1D V.1 | HSCTM-2D V.1 |
|---|---|---|---|---|---|
| FRESHWATER SYSTEMS | | | | | |
| Rivers & Streams: Free-Flowing and Backwater Effects | | | | | |
| Vertically Well-mixed; Laterally Well-Mixed; Narrow & Shallow | ★ | ★ | ★ | ★ | ★ |
| Vertically Well-Mixed; Lateral Gradients; Wide & Shallow | ★ | ★ | ★ | | ★ |
| Vertically Stratified; Laterally Well-Mixed; Narrow & Deep | ★ | ★ | ★ | | |
| Vertically Stratified; Lateral Gradients; Wide & Deep | ★ | ★ | ★ | | |
| Lakes/Bays & Reservoirs | | | | | |
| Vertically Well-mixed; Lateral Gradients; Wide & Shallow | ★ | ★ | ★ | | ★ |
| Vertically Stratified; Laterally Well-Mixed; Narrow & Deep | ★ | ★ | ★ | | |
| Vertically Stratified; Lateral Gradients; Wide & Deep | ★ | ★ | ★ | | |
| SALTWATER/TIDAL SYSTEMS | | | | | |
| Tidal Rivers & Embayments/Lagoons | | | | | |
| Tidal Rivers: Vertically Well-Mixed; Laterally Well-Mixed; Narrow & Shallow | ★ | ★ | ★ | ★ | ★ |
| Tidal Rivers: Vertically Well-Mixed; Lateral Gradients; Wide & Shallow | ★ | ★ | ★ | | ★ |
| Embayments/lagoons: Vertically Well-Mixed; Lateral Gradients; Wide & Shallow | ★ | ★ | ★ | | ★ |
| Estuaries & Coastal Ocean | | | | | |
| Estuaries: Vertically Stratified; Laterally Well-Mixed; Narrow & Deep | ★ | ★ | ★ | | |
| Estuaries: Vertically Stratified; Lateral Gradients; Wide & Deep | ★ | ★ | ★ | | |
| Coastal Ocean: Vertically Stratified or Vertically Well-mixed; Narrow or Wide Shelf | ★ | ★ | ★ | | |

Three-Dimensional: 3D(xy,z). A three-dimensional model is the most physically realistic representation for a waterbody where significant water quality constituent gradients are observed in the longitudinal (x), lateral (y) and vertical (z) dimensions. Relatively deep and large stratified freshwater lakes, reservoirs, bays, estuaries and the coastal ocean are most appropriately modeled with a three-dimensional representation. In a three-dimensional waterbody, none of the three dimensions are considered to be well-mixed since none of the water quality constituent gradients are considered to be negligible in relation to the site-specific problem setting for the analysis.

Evaluation and Comparison of Hydrodynamic Models

In reviewing and evaluating the various features or processes of a hydrodynamic model, the detailed assessment of candidate models focused on (*a*) the capability of a candidate model to represent the appropriate spatial dimensionality, and a key feature, attribute, process or interaction; and (*b*) the level of detail of the formulation(s) used to describe the physical processes or interactions. When the model comparisons are used for selection of a model, the ‘conceptual model’ of the site-specific problem setting will determine which attributes of the ‘head-to-head’ comparisons are the most relevant. The comparison criteria applied for the review and evaluation of hydrodynamic models included the following features and processes:

Spatial Dimensionality
State Variables and Computed Variables
Approximations and Assumptions
Surface and Bottom Boundaries
Vertical stratification
Turbulence Closure
Wetting and Drying
Boundary Conditions and External Forcing Functions
Computational Grid Schemes and Transformations
Numerical Methods for Time-Dependent Solution

The models selected for review and evaluation include the following advanced hydrodynamic models:

CH3D-WES V1.0
ECOM-3D V1.3 and POM
EFDC
EFDC1D
HSCTM-2D V1.0

Table 3.7 presents a summary of the applicability of each hydrodynamic model to the waterbody classifications and spatial dimensionality given in Table 3.6. Table 3.8 presents a comparison of the state variables and computed variables available for each model. Table 3.9 presents a comparison of the approximations, features, processes and numerical methods incorporated in each model.

Spatial Dimensionality

One-Dimensional: 1D(x). Several hydraulic and hydrodynamic models designed for one-dimensional rivers were eliminated from further consideration during screening of our candidate models (see Appendix A). EFDC1D, a modified version of EFDC recently developed for EPA ERD to provide an advanced hydrodynamic model for water quality model applications to a branched network of one-dimensional, variable cross-section streams and rivers (Tetra Tech, 2001), is the only model that is specifically designed for application to one-dimensional freshwater streams and rivers and tidal rivers. CH3D-WES, ECOM-3D, EFDC and HSCTM-2D can all be configured for a one-dimensional waterbody by assigning only one grid cell in the lateral and vertical domains.

Two-Dimensional: 2D(x,y). HSCTM-2D is a two-dimensional, depth-averaged finite element hydrodynamic model that is designed specifically for vertically well-mixed waterbodies such as lakes, shallow estuaries and embayments. RMA-2, a two-dimensional finite element hydrodynamic model developed by Resource Management Associates, is included as the hydrodynamic component of HSCTM-2D. As noted above, HSCTM-2D can also be applied to a one-dimensional freshwater stream or river or tidal river. CH3D-WES, ECOM-3D and EFDC can also be configured for a two-dimensional, depth-averaged waterbody by assigning only a single grid cell in the vertical domain.

Two-Dimensional: 2D(x,z). Stratified, laterally-averaged waterbodies, such as lakes and estuaries that are typically deep and narrow, can be simulated using CH3D-WES, ECOM-3D and EFDC. These advanced models, designed to account for the effect of vertical density gradients on fluid motion, can be applied to these types of waterbodies by configuring a single grid cell in the lateral (y) dimension. EFDC1D and HSCTM-2D can not be applied to a two-dimensional [2D(x,z)] stratified waterbody.

Three-Dimensional: 3D(xy,z). For large waterbodies such as large lakes, reservoirs, rivers, estuaries and the coastal ocean that are strongly stratified and also exhibit pronounced constituent gradients in the horizontal dimensions (xy), CH3D-WES, ECOM-3D and EFDC are appropriate choices for a hydrodynamic model. EFDC1D and HSCTM-2D can not be applied to a three-dimensional waterbody.

State Variables and Computed Variables

Hydrodynamic models provide the (a) velocity and flow fields, (b) elevation of the water surface and (c) bottom stress. The state variables of all the hydrodynamic models include: stage height or free water surface elevation; salinity and velocity. All models except HSCTM-2D also use water temperature as a state variable. As a one-dimensional model [1D(x)], EFDC1D simulates only the ‘u’-component of velocity along the longitudinal (x) direction of flow. As a two-dimensional model [2D(xy)], HSCTM-2D simulates ‘u’ and ‘v’ as the horizontal velocity components. The three-dimensional models, CH3D-WES, ECOM-3D and EFDC simulate velocity in three-dimensions (xy,z) as the ‘u’ and ‘v’ horizontal components and the vertical ‘w’ component. CH3D-WES, ECOM-3D, EFDC and EFDC1D include turbulent kinetic energy and turbulent macroscale length scale parameters as state variables. All of the hydrodynamic models compute water density as a function of at least water temperature and salinity. With the exception of the one-dimensional EFDC1D, all the models compute horizontal diffusivity from horizontal turbulent closure methods as an output variable. CH3D-WES, ECOM-3D and EFDC also compute vertical eddy viscosity and vertical eddy diffusivity from vertical turbulence closure schemes as output parameters of these advanced models.

**Table 3.8. Comparison of State and Computed Variables for Hydrodynamic Models**

| | CH3D-WES V.1 | ECOM-3D V1.3/POM | EFDC | EFDC1D V.1 | HSCTM-2D V.1 |
|---|---|---|---|---|---|
| **Prognostic (State) Variables** | | | | | |
| Stage Height/Free Water Surface Elevation | ★ | ★ | ★ | ★ | ★ |
| Water Temperature | ★ | ★ | ★ | ★ | |
| Salt (Salinity, Chlorides, Specific Conductance, Total Dissolved Solids) | ★ | ★ | ★ | ★ | ★ |
| Velocity: x component (u) | ★ | ★ | ★ | ★ | ★ |
| Velocity: y component (v) | ★ | ★ | ★ | | ★ |
| Velocity: z component (w) | ★ | ★ | ★ | | |
| Turbulent Kinetic Energy | ★ | ★ | ★ | ★ | |
| Turbulent Macroscale (length scale) | ★ | ★ | ★ | ★ | |
| **Computed Variables** | | | | | |
| Density as Function of Salt & Temperature | ★ | ★ | ★ | ★ | ★ |
| Density as Function of Salt, Temperature, Total Suspended Solids & Pressure | | | ★ | ★ | |
| Vertical Eddy Diffusivity | ★ | ★ | ★ | | |
| Vertical Eddy Viscosity | ★ | ★ | ★ | | |
| Horizontal Diffusivity | ★ | ★ | ★ | | ★ |
| **Surface Heat Exchange Forcing Functions** | | | | | |
| Air Temperature | | ★ | ★ | ★ | |
| Dew Point Temperature | | ★ | ★ | ★ | |
| Cloud Cover | | ★ | ★ | ★ | |
| Solar Radiation | | ★ | ★ | ★ | |
| Atmospheric Pressure | | ★ | ★ | ★ | |
| Wind Velocity | | ★ | ★ | ★ | ★ |

<u>Approximations and Assumptions</u>

In all applications of a hydrodynamic model, the length scale of the vertical dimension is typically 2-3 orders of magnitude smaller than the length scale of the horizontal dimension. Since this is the case for all waterbodies, the hydrostatic assumption is invoked for the vertical component of the momentum equation in all the hydrodynamic models evaluated for this study. The Boussinesq approximation, which assumes that density is constant except in the baroclinic terms of the model, is also invoked in all of the models evaluated for this study except for HSCTM-2D. Finally, nearly all hydrodynamic models assume that water is incompressible in a natural water system (Cheng and Smith, 1990).

<u>Surface and Bottom Boundaries</u>

The elevation of the water surface is a key hydrodynamic variable that is used to compute the pressure gradient component of flow in a waterbody (i.e., water flows downhill). Since tidal motions are often of interest in designing hydrodynamic models, a dynamic boundary is applied as a free surface boundary at the air-water surface to allow the water surface to freely move up

**Table 3.9. Features and Approximations of Hydrodynamic Models**

| | CH3D-WES V.1 | ECOM-3D V1.3/POM | EFDC | EFDC1D V.1 | HSCTM-2D V.1 |
|---|---|---|---|---|---|
| **Approximations** | | | | | |
| Incompressible Flow | ★ | ★ | ★ | ★ | ★ |
| Boussinesq Approximation | ★ | ★ | ★ | ★ | |
| Vertical Momentum | | | | | |
| Complete (vertical momentum equation Is solved) | | | | | |
| Hydrostatic Approximation | ★ | ★ | ★ | ★ | ★ |
| **Air-Water Surface Interface** | | | | | |
| Rigid Lid | | | ★ | | |
| Free Surface Boundary | ★ | ★ | ★ | ★ | ★ |
| **Bed-Water Bottom Interface (bottom stress)** | | | | | |
| Linearized | | | | | |
| Quadratic Form: Chezy/Mannings Friction Coefficients | | | | | ★ |
| Logarithmic 'Law of Wall': Roughness Height | ★ | ★ | ★ | ★ | |
| Turbulent Bottom Boundary Layer | ★ | | | | |
| High Frequency Surface Waves | | ★ | ★ | | |
| High Gradient Near Bottom Sediment Concentration | | | ★ | | |
| **Density** | | | | | |
| Well-mixed/homogenous Water Column: Constant Density | | | | ★ | ★ |
| Stratified: Baroclinic (coupled/prognostic; salt & temperature simulated) | ★ | ★ | ★ | | |
| **Turbulence Closure (Horizontal Viscosity/Diffusivity)** | | | | | |
| Constant | | ★ | | | ★ |
| Empirical as Function of Length Scale | | | | | |
| Algebraic/Smagarinsky Sub-grid Scale | ★ | ★ | ★ | ★ | |
| **Turbulence Closure (Vertical Viscosity/Diffusivity)** | | | | | |
| Zero-Equation: Constant | | ★ | | | |
| Zero-Equation: Empirical as Function of Length Scale | | | | | |
| Stability Function Modified by Richardson Number | | | | | |
| One-equation: k Model | | | | | |
| Two-equation: k-e Model | ★ | | | | |
| 2.5-equation: Mellor & Yamada | | ★ | ★ | | |
| **Wetting and Drying** | | | | | |
| Included | | | ★ | | ★ |
| Not Included | ★ | ★ | | ★ | |
| **Boundary Conditions/External Forcing Functions** | | | | | |
| Slip Shoreline/Water Interface | ★ | ★ | ★ | | ★ |
| No-Slip Shoreline/Water Interface | ★ | ★ | ★ | | ★ |
| Semi-Slip Shoreline/Water Interface | | | ★ | | |
| Surface Water Inflow (point source) | ★ | ★ | ★ | ★ | ★ |
| Surface Water Distributed Inflow (nonpoint source) | ★ | ★ | ★ | ★ | ★ |
| Groundwater Inflow (nonpoint source) | | | ★ | ★ | |

**Table 3.9. Features and Approximations of Hydrodynamic Models (concluded)**

| | CH3D-WES V.1 | ECOM-3D V.1.3/POM | EFDC | EFDC1D V.1 | HSCTM-2D V.1 |
|---|---|---|---|---|---|
| **Boundary Conditions/External Forcing Functions (concluded)** | | | | | |
| Salt Inflow | ★ | ★ | ★ | ★ | ★ |
| Water Temperature (Heat) Inflow | ★ | ★ | ★ | ★ | |
| Evaporation | ★ | ★ | ★ | ★ | |
| Precipitation Input | ★ | ★ | ★ | ★ | |
| Tides/Water Surface Elevation at 'Clamped' /'Fixed' Open Boundary | ★ | ★ | ★ | ★ | ★ |
| Free Radiation Open Boundary[1] | ★ | ★ | ★ | ★ | |
| **Coriolis 'Force' (large open w ater systems)** | | | | | |
| Included | ★ | ★ | ★ | | ★ |
| Not Included | | | | ★ | |
| **Horizontal (xy) Grid Scheme/Coordinate Transformation** | | | | | |
| Cartesian (no transformation) | ★ | ★ | ★ | ★ | |
| Algebraic | | | | | |
| Curvilinear/Orthogonal | | ★ | ★ | | |
| Boundary Fitted/Curvilinear/Non-Orthogonal | ★ | | | | |
| Quadrilateral Elements | | | | | ★ |
| **Vertical (z) Grid Scheme/Coordinate Transformation** | | | | | |
| Cartesian | | | | | |
| 'z-Plane' | ★ | | | | |
| Sigma-Stretched Grid | ★ | ★ | ★ | | |
| **Horizontal (xy) Numerical Solution Method** | | | | | |
| Finite Difference | ★ | ★ | ★ | ★ | |
| Finite Element | | | | | ★ |
| **Vertical (z) Numerical Solution Method** | | | | | |
| Finite Difference | ★ | ★ | ★ | ★ | |
| Finite Element | | | | | |
| **Time Stepping Numerical Solution Method** | | | | | |
| Explicit | | ★ | | | ★ |
| Fully Implicit | | | | | ★ |
| Semi-implicit | ★ | | ★ | ★ | ★ |
| Internal-External Mode Splitting | ★ | ★ | ★ | | |

**footnotes**

**1** Specification of the open w ater boundary condition for a hydrodynamic model is difficult because of the the transient nature of the numerical solution. Unless the appropriate boundary conditions for the interface betw een the model domain and the open w ater boundary are specified, the model simulates an artificial w ave disturbance or "noise" reflected w ithin the model domain that does actually exist. A simple physical analogy for a 'clamped' or 'fixed' radiation boundary condition is the reflection of the transient vibrations propagated by plucking a guitar string or striking a drum head. The backw ater effect of a dam on flow in a river or a w ind driven seiche in a large lake are examples w here a 'clamped' or 'fixed' radiation boundary in a hydrodynamic model is an appropriate description for the boundary. The 'clamped' boundary condition controls the w ater surface elevation at the boundaries of the domain. To accurately simulate the physical conditions that actually occur near the open w ater boundary of a model domain for coastal seas, the free radiation boundary condition must be used to allow the transient w ave disturbance simulated by the model to pass through a 'transparent' or 'non-reflecting' boundary.

or down in response to tides and winds. All the hydrodynamic models evaluated for this study allow a free surface boundary. EFDC also includes a rigid lid boundary option that is appropriate for models of large open water systems such as very large lakes or the open ocean; in these large bodies of water, the typical change in surface elevation is very small relative to the depth of the water column

At the water-sediment bed boundary, fluid motion over the bed results in bottom stress. Bottom stress formulations that define the rate of momentum loss at the water-sediment bed boundary are a feature that allows one to differentiate between hydrodynamic models. HSCTM-2D employs the quadratic form of the 'Chezy-Mannings' friction coefficient. A user-defined roughness height is used in the logarithmic 'law of the wall' in CH3D-WES, ECOM-3D, EFDC and EFDC1D. CH3D-WES also provides an optional turbulent bottom boundary layer formulation to define bottom stress. ECOM-3D and EFDC both allow high frequency surface waves to be incorporated as terms in the bottom stress formulations.

<u>Vertical Stratification</u>

Approximations related to the relative strength, or weakness, of vertical stratification in a water body, and its influence on the vertical flux of horizontal momentum, allow differentiation between hydrodynamic models. In shallow water bodies, such as broad lakes, reservoirs and embayments, that can be considered well-mixed, the weak conditions of vertical stratification allow a strong coupling of surface wind stresses and bottom friction stresses on circulation within the interior of the water column. A two-dimensional, depth-averaged [2D(xy)] hydrodynamic model is thus appropriate for a well-mixed water body that eliminates the influence of vertical density gradients on the horizontal pressure field. The baroclinic component of the equations of fluid motion (i.e., the terms that describe how dense water sinks) are not included in a depth-averaged model. HSCTM-2D is specifically designed as a two-dimensional (horizontal) model for application in shallow, well-mixed waterbodies. With the assignment of a single grid cell in the vertical dimension, CH3D-WES, ECOM-3D and EFDC can also be applied to shallow, well-mixed waterbodies.

In stratified waterbodies, the force component resulting from vertical density gradients in a strongly stratified body of water is about two orders of magnitude less than the forces arising from surface winds and bottom friction. The relative strength, or weakness, of stratification of the water column (i.e., stability) is described by the Richardson number as the ratio of buoyancy to mixing energy from turbulent shear stress. The Richardson number thus provides an index of the tendency of the water column to either mix (weak stratification) or resist mixing (strong stratification). Large values of the Richardson number indicate strong stratification while very small values are indicative of weakly stratified, well-mixed conditions. Under conditions of strong stratification, little vertical exchange of momentum, salt, heat or other dissolved constituents takes place. As a result of strong stratification in lakes, reservoirs, estuaries and coastal waters, for example, significant depletion of dissolved oxygen can occur in the near bottom layer since the mixing of atmospheric oxygen across the air-water interface from the surface layer through the water column to the bottom is restricted at a depth in the water column defined by the strongest vertical gradients of water temperature (thermocline), salinity (halocline) and density (pycnocline). In contrast to a depth-averaged model, the baroclinic component of the equations of fluid motion must be included in a model of stratified waterbodies. CH3D-WES, ECOM-3D and EFDC, all designed to compute the vertical density gradient, can be applied for hydrodynamic studies of stratified two- and three-dimensional waterbodies.

Turbulence Closure

Functional relationships to describe horizontal and vertical turbulent mixing, defined as the turbulence closure problem, are needed in hydrodynamic models because of the introduction of an additional variable to represent turbulent mixing in the time-averaged equations of motion. Turbulence closure formulations are differentiated in hydrodynamic models by the number of equations used to define turbulent mixing coefficients as: (a) constant empirical or zero-order; (b) one-equation, (c) two-equations and (d) higher order methods. Hydrodynamic models can thus be differentiated by the methods used to define horizontal and vertical turbulent mixing.

In addition to the influence of turbulent shear stresses on the weakness or strength of stratification of the water column, turbulent exchange of momentum, heat and mass is considered in hydrodynamic models by time averaging the instantaneous terms of the equations of motion that account for the random fluctuations of fluid motion generated by molecular diffusion and small scale differences in velocity in the horizontal and vertical dimensions. In hydrodynamic and mass transport models, the sub-grid scale influence of turbulent mixing is parameterized using horizontal and vertical eddy diffusivity coefficients.

Constant. The simplest approach adopted in hydrodynamic and mass transport models is to represent turbulent mixing processes using empirical relationships determined from field experiments to specify a constant mixing coefficient. For large lakes and oceans, observations (e.g., Okubo, 1971) demonstrate that empirical estimates of horizontal eddy diffusivity can be functionally related to the length scale of turbulence to the ‘4/3' power. For a numerical model, the horizontal eddy diffusivity can be reasonably estimated using the length dimensions of the computational grid cells. HSCTM-2D and ECOM-3D allow the specification of a constant length-scale dependent mixing term to describe horizontal turbulence.

Parameterization of the effect of turbulent mixing in the vertical dimension of a water column, although also dependent on length scales, is considerably more complex than the fairly straightforward ‘4/3' power relationship for horizontal eddy diffusion. Using vertical profiles of density and calculations of the local gradient Richardson number, empirical estimates of vertical eddy diffusion can be derived using an approach first described by Munk and Anderson (1948). Martin and McCutcheon (1999) present a lengthy compilation of the Munk and Anderson class of empirical relationships that have been reported in the literature. Using a length scale approach similar to that developed for horizontal mixing, estimates of vertical diffusion coefficients have been functionally related to the thickness of the thermocline layer in lakes (see Chapra, 1997). ECOM-3D is the only three-dimensional model that allows the option to use a constant length-scale dependent mixing term to describe vertical turbulent mixing.

One-Equation. Rather than the external parameterization (i.e., assign zero-order values) of horizontal and vertical eddy diffusion coefficients, more complex one-equation and two-equation approaches have been applied in hydrodynamic models to internally derive turbulent mixing coefficients. One-equation methods of turbulence closure relate eddy coefficients to turbulent kinetic energy and an empirically assigned length scale. None of the models reviewed provide a ‘one-equation’ model as an option for describing turbulence.

Two-Equations. CH3D-WES, ECOM-3D and POM, EFDC and EFDC1D use the algebraic Smagarinsky sub-grid scale scheme for computing horizontal turbulent mixing. Two-equation methods expand on the one-equation approach by adding a second equation to determine the mixing length scale. Advanced hydrodynamic models, in use since the mid-1980s, such as ECOM-3D and POM, CH3D-WES and EFDC employ two-equation closure methods to provide internal calculations of vertical eddy diffusivity. CH3D-WES uses the 2 equation 'k-e' model while ECOM-3D and EFDC use the 2.5 equation 'Mellor &Yamada' formulation.

Wetting and Drying

The cyclic wetting and drying of the shallow portion of an embayment is a common occurrence for a tidally driven system. In freshwater rivers, flood conditions also result in a wetting and drying situation from inundation and recession over the floodplain. Three-dimensional models that do not allow for wetting and drying avoid the problem by defining the 'shoreline' boundary as the depth contour that marks the always wet 'deep' portion of a tidal embayment. The 'bankfull' elevation of a river is defined as the shoreline boundary for a river model if inundation of water and solids onto the floodplain is not a feature of the 'conceptual model' for the problem setting. The versions of CH3D-WES and ECOM-3D reviewed for this study do not include wetting and drying as features of these models. EFDC and HSCTM-2D do include wetting and drying as a feature to allow a portion of the model domain to be alternately wet and dry from either tidal cycling or floods conditions.

Boundary Conditions and External Forcing

Hydrodynamic models must be properly designed to represent the boundary influences of the solid shoreline and open water on the simulation of water surface elevation and velocity within the interior domain of the model. The type of boundary conditions that can be defined for a model control the influence of the boundaries on the interior solution.

'Slip' and 'No-Slip' Boundary. At the shoreline boundary of a waterbody, the components of velocity, viscosity and diffusivity normal to the shoreline are set to zero for the 'no-slip' boundary condition. The 'no-slip' boundary condition is used in CH3D-WES, ECOM-3D, EFDC and HSCTM-2D. The 'no-slip' condition is not relevant for EFDC1D since the direction of one-dimensional flow is parallel to the river banks. The 'slip' boundary condition is available as an option in CH3D-WES, ECOM-3D, EFDC and HSCTM-2D. EFDC also allows a 'semi-slip' boundary condition to be specified.

'Clamped' and 'Free' Radiation Boundary. Specification of open water boundary conditions for a hydrodynamic model is often problematic. In designing the hydrodynamic model domain, the boundaries should be delineated at a sufficient distance away from the interior so that the effect of the boundaries does not influence the solution within the interior domain. In a large model domain, the boundary effects may be minor. In a smaller model domain, however, the specified time-varying boundary conditions of flow and water surface elevation over-specify or 'clamp' the boundary causing artificial interactions, or transient noise, between the boundary and the interior flow. This artificial disturbance occurs because the reflection of the waves does not actually exist. The accurate simulation of the open water boundary condition requires a 'free' radiation boundary condition that allows the transient wave disturbances to pass through a non-reflecting boundary. In contrast to an open water boundary where the 'free' radiation boundary condition is needed, the 'clamped' or 'fixed' boundary is an appropriate description when the outflow across the boundary is controlled by astronomical tides, or dams, impoundments and other flow control structures. The effects of a wind-driven, oscillating seiche in a lake (e.g., Lake Michigan) is another example where a 'clamped' boundary (i.e., the elevation of the opposite shoreline) is an appropriate boundary condition. All the models include the option to specify a 'clamped' boundary condition to control the water surface at the boundaries of the model domain. CH3D-WES, ECOM-3D, EFDC, and EFDC1D also include the option to specify a 'free' radiation boundary condition for open water systems. HSCTM-2D is the only model that does not include the 'free' radiation boundary condition.

External Forcing Functions. All the models include the capability to input time-series of freshwater, salt and heat inflows to define the input from tributaries, wastewater discharges and watershed runoff. EFDC is the only model that includes the capability to specify groundwater inflow through the sediment bed across the sediment-water interface. Meteorological time-series that can be input to CH3D-WES, ECOM-3D, EFDC and EFDC1D include evaporation and precipitation. ECOM-3D, EFDC, and EFDC1D provide the capability to input time-series of air and dew point temperature, cloud cover, solar radiation, atmospheric pressure and wind velocity. HSCTM-2D provides for the input of wind velocity time-series.

Computational Grid Schemes and Transformations

Although circulation in a waterbody is largely controlled by winds, tides, freshwater inflow and density gradients, water motion is also influenced by geometry of the shoreline and the bottom contours. In order to construct an accurate hydrodynamic simulation, the computational grid representation of the shoreline and the bottom contours must be as realistic as possible for the numerical solution of the spatial terms of the equations of motion. Numerical solution techniques for horizontal grids include finite-difference methods and finite-element methods.

Horizontal Transformations. A rectangular cartesian grid (i.e., checkerboard) is the simplest method to represent the shoreline and bottom boundary of a waterbody to map the computational grid domain for a finite-difference numerical solution. In an open water system, where the shoreline is not considered and the bottom slope is moderate, a rectangular cartesian grid is appropriate for the numerical grid of a model. In an enclosed waterbody, however, where the shoreline and the bottom contours are highly irregular, the use of a rectangular cartesian grid introduces artificial vorticities and gyres because of the 'staircase' grid cells that represent water but intersect the shoreline or the bottom (Sheng, 1990). This is the problem that motivated the development of finite-element grid models where the computational grids are defined by a mesh of triangles or rectangles where the sizes of the triangles and rectangles are scaled to match the irregular geometry of the shoreline. Finite-difference methods are retained, however, by following irregular shoreline geometry and bathymetry with the construction of curvilinear grid schemes that are transformed to a rectangular grid for a finite-difference solution. A curvilinear grid is used to avoid the artificial numerical results caused by a 'staircase' cartesian grid scheme. The modeler has the choice of constructing a curvilinear coordinate grid as (a) orthogonal or (b) boundary fitted non-orthogonal.

All the models are designed to accommodate a rectangular cartesian coordinate system. ECOM-3D and EFDC use an orthogonal curvilinear coordinate scheme. CH3D-WES is the only model that uses a boundary fitted non-orthogonal curvilinear grid scheme. As the only finite-element model, HSCTM-2D defines the computational domain of a waterbody using either linear or quadratic quadrilateral or triangular elements to follow the irregular shoreline of a well-mixed waterbody. Quadratic elements allow for the sides of the elements to be curved to better approximate the shoreline shape.

Vertical Transformations. Similar to the horizontal grid schemes, a rectangular cartesian coordinate system is the simplest approach to implement in a model. Rectangular cartesian coordinates are satisfactory for a waterbody characterized by relatively flat bottom topography. For a waterbody characterized by either sloping or irregular bottom contours, a cartesian coordinate scheme can result in vertical 'staircase' grid cells and the introduction of artificial vorticity in the numerical solution. A sigma-stretched bottom following vertical coordinate scheme is adopted in CH3D-WES, ECOM-3D and EFDC to avoid the numerical problems associated with rectangular 'staircase' grid cells. A sigma-stretched vertical grid retains the same number of vertical layers (e..g., 5-10 layers) throughout the entire spatial domain of the model. The thickness of each vertical layer for each grid cell is variable since the thickness is computed from the number of vertical layers and the water column depth assigned to each surface layer grid cell. Applications of hydrodynamic models based on the 'sigma-stretched' coordinate system have resulted in problems related to the simulation of density interfaces in physical domains characterized by sharp gradients of bathymetry. Initial applications of the 'sigma-stretched' version of CH3D resulted in numerical problems with density simulations in the region of the 'deep trench' in Chesapeake Bay. An alternate approach used only in CH3D-WES to overcome this computational problem is the 'z-plane' vertical coordinate system.

Numerical Methods for Time-Dependent Solution

Numerical integration techniques are classified as either explicit, semi-implicit or fully implicit methods. Explicit finite-difference integration schemes are simple to code and implement in a model. Explicit methods, however, introduce numerical dispersion into the solution and the Courant-Friederichs-Levy (CFL) criterion for numerical stability limits the computational time step to a very small value. The computational burden of an explicit scheme is thus large. Alternative approaches to explicit methods include semi-implicit and fully implicit finite-difference integration schemes. These schemes, although more complex from a computational perspective than explicit methods, are more efficient since a longer time step can be used than the small time steps required for explicit schemes. ECOM-3D and HSCTM-2D use explicit methods for the time integration schemes. HSCTM-2D also employs semi-implicit and fully implicit schemes. CH3D-WES, EFDC, and EFDC1D use semi-implicit methods.

The fluid equations that govern circulation dynamics include terms that define the propagation of fast moving external free surface gravity waves (barotropic mode) and internal shear (baroclinic mode) from slow moving internal gravity waves. For reasons of computational efficiency, the vertically integrated (external barotropic mode) equations are solved separately from the vertically dependent (internal baroclinic mode) equations. This technique, used by CH3D-WES, ECOM-3D and EFDC, is known as internal-external mode-splitting for the time-stepping numerical integration scheme. In this mode-splitting technique, small time steps can be used in the external mode while larger time steps are used in the internal mode. The overall effect of the mode-splitting technique is to improve computational efficiency of a hydrodynamic model.

### 3.3 Evaluation of Model Support and Usability

This section provides information on several key elements that together make up what is commonly called "model support". For this effort, model systems (i.e., entire software suites that include many components) were investigated. Whenever possible, this evaluation was performed for "modeling systems" rather than modeling components. Generally speaking, the nature and quality of model support and usability is shared among its modeling components. However, it was not a requirement of this study that components included in any one of the groups that were evaluated be linked, either internally or externally, to components of *all* other groups. Table 3.10 identifies the relationships between all components that were included in the detailed comparison performed for this study. Internet access to the models and/or the documentation for each is also listed in Table 3.10 under the *url* column.

Table 3.10 Modeling Systems and/or Components included in the Model Support Comparison

| System | Hydro-dynamics | Sediment | Toxic Chemicals | Conventional Pollutants | URL |
|---|---|---|---|---|---|
| AQUATOX | | | AQUATOX | AQUATOX | http://www.epa.gov/waterscience/wqm/ |
| CE-QUAL-ICM | CH3D-WES | | | CE-QUAL-ICM | http://smig.usgs.gov/smic/ |
| ECOMSED | ECOM-3D | ECOMSED | | | www.hydroqual.com |
| EFDC | EFDC | EFDC | EFDC | EFDC | http://smig.usgs.gov/smic/ |
| EFDC1D | EFDC1D | EFDC1D | EFDC1D | EFDC1D | (none identified) |
| HSCTM-2D | HSCTM-2D | HSCTM-2D | HSCTM-2D | | http://www.epa.gov/ceampubl/swater/index.htm |
| HSPF | | HSPF-RCHRES | HSPF-RCHRES | HSPF-RCHRES | http://water.usgs.gov/software/hspf.html |
| IPX 2.7.4 | | IPX 2.7.4 | IPX 2.7.4 | | (none identified) |
| WASP5(6) | EFDC, DYNHYD | WASP5(6)-TOXI5(6) | WASP5(6)-TOXI5(6) | WASP5(6)-EUTRO5(6) | http://smig.usgs.gov/smic/<br>http://www.epa.gov/waterscience/wqm/ |

Model support can be characterized as consisting of the following four basic elements: documentation, model application aids, human support, and model usage attributes.

## Documentation

It was a requirement for models evaluated in this study that their documentation and user instructions be available either in printed form or as an interactive resource embedded in the model package itself. User instructions on input and output operations for the current release must be available, as well as documentation of the model's governing equations, their transformation to solvable forms, and any supporting algorithms. Model documentation must also make clear the limitations and the environmental conditions under which the model can be appropriately applied.

Each model was evaluated for the existence, availability and general quality of documentation, including the user's manual, discussion of theory, and coding structure. Specifically, the primary user's manual document was identified, consistent with the model version release under consideration, and evaluated the clarity and completeness of the documentation. The discussion of theory pertinent to application of the model's features was examined, and an evaluation was made of to what extent the coding structure presented would support thoughtful application of the model.

## Application Aids

Review of model user's manuals and selective interviews with model developers/maintenance providers were performed to determine whether or not modeling techniques/tools (e.g., graphical user interfaces, pre- and post-processors, linkage capabilities to GIS) intended to enhance ease-of-use were available for models. Specifically, the availability of a graphical user interface, the availability and completeness of pre- and post-processors, whether the post-processor handles field data to model data comparisons, and whether the model is linked to a geographical information system (GIS) were evaluated.

Human Support

It was also a requirement for models evaluated in this study that technical support be readily available for the model; support may be provided via telephone, Internet correspondence or personal contact, and need not be provided without fee.

Accordingly, the degree of application support available was evaluated. It was determined whether assistance in applying the model is available from the developer or sponsor and/or additional sources. User's groups, web sites and list servers, and recurring conferences, workshops, and symposia were also been identified.

Model Usage

An additional requirement of models evaluated in the study was that each model have a proven track record of successful applications to real world problems. One of three criteria must be met. Either (1) an application of the model must have undergone peer review by an expert (or panel or experts) with the results of the review published in the open literature, or (2) an application of the model must have been published in a peer-reviewed journal, or (3) the model 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 usage analysis that was developed has two components. First, a general assessment of each model's application history was perfromed. Second, the resource requirements (level of effort, data requirements, user expertise) for applying each model were assessed. The level of effort and user expertise is admittedly a subjective evaluation. The level of effort and data requirements are highly correlated since much of the effort in applying a model is gathering data and building an input data set. Since all the models require kinetics coefficients as well as time series data of all boundary conditions and forcing functions, the data requirements are strongly influenced by the number of constituents being modeled and the dimensionality of the model. The level of effort is influenced by the organization, completeness, and accuracy of the user's manual, the format of the input data file and the availability of pre- and post-processors and other model application aids. Required user expertise is largely a function of the complexity of the contaminated sediment scheme.

### 3.3.1 AQUATOX (Release 2.0)

Overview

Release 2.0 of AQUATOX is an advanced, dynamic, process-based aquatic ecosystem model that integrates principles of aquatic ecology, chemical dynamics, contaminant bioaccumulation and ecotoxicology for assessments of ecological risk. Using finite difference methods for numerical solution, AQUATOX simulates the transport and fate of dissolved oxygen, inorganic and organic carbon and nutrient cycles with trophic level processes and interactions of algae, benthic algae, submerged macrophytes, zooplankton, invertebrates and fish within the water column and the sediment bed.. AQUATOX has been applied to single reaches of streams and rivers as a completely mixed model (0-D) and ponds, lakes and reservoirs as a vertical two-layer model [1D(z)] of the epilimnion and hypolimnion.

Version 3.0 of AQUATOX, not yet available from EPA, will provide the capability to represent streams, rivers, ponds, lakes, reservoirs and tidal rivers and embayments as a multi-dimensional system of interconnected spatial segments where the dimensionality is defined as 1D(x), 2D(x,y), 2D(x,z) or 3D(xy,z). Version 3.0 will also include the capability to represent deposition and resuspension of solids using a multiple bed layer model similar to that incorporated in IPX Version 2.7.4 (Velleux et al., 2001). An estuarine version of AQUATOX has also been developed and calibrated for Galveston Bay, Texas. The bioaccumulation module of the estuarine version has been validated with data from New Bedford Harbor in Massachusetts.

Hydrodynamics

AQUATOX does not include an internal hydrodynamic model. Time-dependent hydraulic data is provided externally by the modeler as input data to assign flow, velocity, surface elevation and/or depth, surface area, cross-sectional area and volume of the waterbody. AQUATOX is an integral part of EPA's 'BASINS' modeling system and is linked to HSPF. The hydrodynamic and bathymetric data needed for input to AQUATOX is provided by HSPF.

Sediment Transport

Release 2.0 of AQUATOX includes an internal sediment transport model that has been recently verified against results generated by the sediment transport model of HSPF-RCHRES. Data needed to characterize the settling, deposition and resuspension properties of the three classes of inorganic solids (clays, silts and sands) included in AQUATOX is assigned by the modeler as input data.

Toxic Chemicals Transport and Fate

Release 2.0 of AQUATOX provides simulations of the transport pathways and fate of multiple toxic chemicals within the water column, sediment bed and aquatic food web. Within the water column and the bed, reactions related to hydrolysis, photolysis, volatilization, oxidation and biodegradation are included as kinetic processes. AQUATOX also accounts for equilibrium and non-equilibrium partitioning of toxicants within the water column and the bed to inorganic solids and the dissolved and particulate fractions of organic matter. AQUATOX represents bioaccumulation and biotransformation as well as the toxicity effects of toxicant(s) within the aquatic food web.

Conventional Pollutants and Eutrophication

Release 2.0 of AQUATOX provides the capability to simulate the transport and fate of dissolved oxygen, organic matter and nutrients (N,P) as components of a complex representation of multiple trophic levels of an aquatic food web. Organic matter is represented using labile and refractory fractions of dissolved and particulate organic matter. Multiple functional groups of planktonic algae (e.g., greens, diatoms, dinoflagellates), benthic algae and submerged macrophytes can be represented as primary producers with secondary, and higher, order producers included as components of a complex aquatic food web. The coupling of the deposition of particulate organic matter to the sediment bed with sediment oxygen demand and benthic nutrient release across the sediment-water interface is internally simulated using a simplified model of organic matter decomposition and remineralization in the sediment bed.

Documentation

The documentation package that was reviewed includes AQUATOX for Windows, Release 2 (Park and Clough, 2002), AQUATOX for Windows, Release 1, which consists of Volume 1 User's Manual (USEPA, 2000a), Volume 2 Technical Documents (USEPA, 2000b), and Volume 3 Model Validation Reports (USEPA, 2000c) with addendum Release 1.1 (USEPA, 2001). The documentation contains an extensive discussion of theory in Volume 2. The model's coding structure is presented as a diagram of computation modules. Executable model files have been identified and are available, but the source code is not.

Application Aids

A graphical user interface is available – AQUATOX for Windows. The pre-processor generates input data; the post-processor generates output figures and difference plots. AQUATOX is associated with BASINS, but GIS linkage has not been implemented for this model.

Human Support

Support can be found at EPA Office of Water Programs, EPA Office of Pollution Prevention & Toxics (OPPT) and EPA OST. EPA will send email messages to registered users with updates and future releases.

No workshops, web-sites, list server user groups, or recurring conferences or symposia are identified.

Model Usage

There are four case studies provided in Volume 3 of the documentation: Lake Onondaga, NY; Coralville Reservoir, IA; Lake Ontario; and Walker Branch, TN. These validation and calibration studies were completed by the model authors on evolving versions of the model which had only very minor differences from the release version.

Level of Effort - Moderate to High. As is the case for all models in this evaluation, the level of effort depends on the application.
Data Requirements – Moderate. Non-dimensional, point model.
User Expertise – Moderate. Typical for this type of model and dependent on the application. Some interpretation may be required for generating input and evaluating output.

### 3.3.2 CE-QUAL-ICM (Release 1.0)

Overview

CE-QUAL-ICM, an advanced water quality model for conventional pollutants and eutrophication, was developed by the U.S. Army Corps of Engineers, Waterways Experiment Station for EPA's Chesapeake Bay Program. CE-QUAL-ICM is a finite difference model that can be applied for multi-dimensional waterbodies as 1D(x), 2D(x,y), 2D(x,z) and 3D(xy,z) representations. This advanced model includes 22 state variables to represent algae, organic carbon, nutrients and dissolved oxygen. CE-QUAL-ICM has been applied to Chesapeake Bay, the Delaware Inland

Bays, the New York Bight, New York Harbor, Long Island Sound, Lower Green Bay, Florida Bay and other estuarine systems.

Hydrodynamics

CE-QUAL-ICM does not include an internal hydrodynamic model. The data needed to specify segment volumes, flow and diffusion coefficients are provided externally as input data to the model. For applications to complex waterbodies, CE-QUAL-ICM is linked with a separate advanced hydrodynamic model such as CH3D-WES. CH3D-WES (Curvilinear Hydrodynamics in a 3-Dimensions-Waterways Experiment Station) is an advanced, time-dependent three-dimensional hydrodynamic model that provides simulations of water temperature, salinity, water surface elevations and the velocity/ flow field (Sheng, 1990; Johnson et al., 1991; 1993). All the major physical processes that govern the barotropic and baroclinic components of water motion and mixing in natural waters are considered in CH3D-WES. Turbulent closure formulations are incorporated in the model to provide internal simulations of horizontal and vertical diffusion processes. CH3D-WES is designed to represent a finite difference computational grid as either a simple cartesian grid or a boundary-fitted, curvilinear coordinate system for irregular complex shorelines. In the vertical domain, CH3D-WES can use either a ‘z-grid’ or a ‘sigma-stretched-grid’ to represent complex bathymetry.

Sediment Transport

CE-QUAL-ICM does not include an internal sediment transport model. Time-and space-dependent settling velocities of particulate organic matter and algae are assigned externally as input data to the model. CE-QUAL-ICM/TOXI, developed by the U.S. Army Corps of Engineers, Waterways Experiment Station as a framework for the transport and fate of solids and toxic chemicals, incorporates advanced sediment transport formulations the water column and the sediment bed. CE-QUAL-ICM/TOXI is not, however, currently available in the public domain as of March 2003 since it is considered to be under active development by the Waterways Experiment Station. See Section 3.1.2 for a description of CE-QUAL-ICM/TOXI.

Toxic Chemical Transport and Fate

CE-QUAL-ICM does not include an internal toxic chemicals transport and fate model. Toxicity effects from toxic chemicals on biological processes are not represented in CE-QUAL-ICM. CE-QUAL-ICM/TOXI, not yet available in the public domain, accounts for multiple toxic chemicals and multiple classes of solids. CE-QUAL-ICM/TOXI is not available in the public domain as of March 2003 since the model is considered to be under development by the Waterways Experiment Station. See Section 3.1.2 for a description of CE-QUAL-ICM/TOXI).

Conventional Pollutants and Eutrophication

CE-QUAL-ICM is an advanced eutrophication model that incorporates multiple functional groups of planktonic algae, dissolved oxygen, nutrient cycles of nitrogen, phosphorus and silica, organic carbon, chemical oxygen demand and total active metal as the 22 state variables of the model. Organic carbon and organic nutrients are represented as dissolved and particulate labile and refractory forms. The predictive sediment diagenesis model of Di Toro (2000) is incorporated in CE-QUAL-ICM to internally couple the deposition of particulate organic carbon to the sediment bed with sediment-water fluxes of inorganic nutrients and dissolved oxygen.

## Documentation

The documentation we reviewed is titled "User's Guide to the CE-QUAL-ICM Three-dimensional Eutrophication Model, Release Version 1.0" (Cerco and Cole, 1995). It consists of 320 pages. The manual is clear and complete. There is an extensive discussion of theory. The model's coding structure is presented as a flowchart with subroutine descriptions. The FORTRAN code is available.

The manual is well organized with introductory material to allow the first time user to set up and run the model with a minimum of outside support. Each constituent modeled is described in a separate section where all the processes which affect it are described and represented by equations and materials flow diagrams. The construction of a data set is described in detail and extensive cross-referencing makes it convenient for the user to refer back to the kinetic equations while inputting data. The manual is detailed enough to help the experienced user take full advantage of the model's capabilities. The only suggestion for substantive improvement would be providing an overall materials flow diagram to help the first time user understand the interactions of the state variables in the water quality model. The toxic routines are from EPA's WASP5 model.

## Application Aids

Model Application Tools - None identified.
Linkage to GIS was not identified. A graphical user's interface is not identified. Pre-processing can be done using SMS third party software. No post-processing was identified. Field data – model data comparisons abilities were not identified.

## Human Support

Model distribution: www.wes.army.mil/el/elmodels/

User's Groups - None identified.
The US Army Waterways Experiment Station (WES) can provide support for a fee.

Conferences, Workshops, Symposia, web sites, or list server users groups were not identified.

## Model Usage

This model was used in conjunction with a hydrodynamic model and a benthic-sediment model to develop a state-of-the-art 3-D model of the Chesapeake Bay. The model was employed to simulate long-term eutrophication trends in Chesapeake Bay. Other applications since the early 1990's include an assessment of the water quality impacts of a confined disposal facility in Green Bay, Wisconsin; effects of benthic algae on eutrophication in Indian River - Rehoboth Bay Delaware; and impact of a flood-diversion tunnel on Newark Bay and adjacent waters, New York Bight, and 7 other applications.

Level of Effort - Moderate to high. The availability of non-proprietary pre- and post-processors would reduce this effort.

Data Requirements - Moderate to high. Typical for this type of model and dependent on the application. Some interpretation may be required for generating input and evaluating output.

User Expertise - High due to a eutrophication scheme with up to 18 state variables and a complex sediment diagenesis model.

### 3.3.3 ECOMSED (Version 1.3)

Overview

The Estuarine Coastal Ocean Model-Sediment (ECOMSED) is a time-dependent, three-dimensional model developed by HydroQual, Inc. to interface an advanced hydrodynamic model (ECOM) with an advanced sediment transport model (SEDZL) for application to rivers, lakes, reservoirs, tidal rivers, estuaries and coastal systems. ECOMSED has its origins in the Princeton Ocean Model (POM) developed by Blumberg and Mellor (1987) for hydrodynamic simulations and SEDZL developed by Ziegler and Lick (1986) and Ziegler et al. (1990) at the University of California-Santa Barbara.

ECOMSED is designed to represent a finite difference computational grid as either a simple cartesian grid or an orthogonal, curvilinear coordinate system for irregular coastlines. In the vertical domain, ECOM uses a 'sigma-stretched-grid' to represent complex bathymetry. ECOM and/or ECOMSED has been applied to numerous waterbodies including New York/New Jersey Harbor and the New York Bight, Green Bay (Wisconsin), Chesapeake Bay, the Upper Mississippi River, Massachusetts Bay, the Hudson River, the Yellow Sea (China), Lavaca Bay (Texas), and the Gulf of Mexico.

Hydrodynamics

The ECOM model used for hydrodynamic simulations is based on the Princeton Ocean Model (POM) (Blumberg and Mellor, 1987). ECOM and/or the POM are used by hundreds of government agencies, academic research groups and consulting firms worldwide. Similar to other modern hydrodynamic models, all the major physical processes that govern the barotropic and baroclinic components of water motion and mixing in natural waters are considered in ECOM. Prognostic state variables of ECOM include water temperature, salinity, water surface elevations and the 3D velocity/ flow field. Turbulent closure formulations are incorporated in the model to provide internal simulations of horizontal diffusion and vertical diffusion processes.

Sediment Transport

The sediment transport model of ECOMSED, SEDZL, is an advanced sediment transport model that has been applied for numerous studies in rivers (Ziegler and Nisbet, 1994), large lakes, reservoirs (Ziegler and Nesbit, 1995) and coastal waters. This advanced model is designed to internally simulate settling, deposition and resuspension of single classes of cohesive and non-cohesive particles using advanced formulations based on the most recent research findings. Water column and bed exchange of particles is represented as functions of bed shear stress and bed shear strength for cohesive solids and the 'Shields' parameter for non-cohesive solids. Consolidation of the sediment bed is represented by a surface bed layer and multiple deep bed layers that respond to accumulation or erosion of solids from the bed.

Toxic Chemical Transport and Fate

ECOMSED does not include an internal toxic chemicals transport and fate model. RCA-TOX, not yet available in the public domain from HydroQual, Inc., accounts for multiple toxic chemicals and cohesive and non-cohesive classes of solids. See Section 3.1.2 for a description of RCA-TOX.

Conventional Pollutants and Eutrophication

ECOMSED does not include an internal eutrophication model. RCA, an advanced eutrophication model that is not yet available (as of March 2003) in the public domain from HydroQual, Inc., accounts for multiple algal groups, nutrients, organic carbon and an internally coupled sediment diagenesis model. See Section 3.1.2 for a description of RCA.

Documentation

The documentation that was reviewed is titled “A Primer for ECOMSED. Version 1.3” (HydroQual, Inc., 2002). It consists of 188 pages, with 55 pages of theory discussion. The coding is presented with a framework figure, flowcharts, and a chapter titled “Structure of Computer Code” in the primer. The source code is in the public domain.

Application Aids

A graphical user interface for this version of the model is not available, but a complete pre- and post-processor is under development. Currently, pre-processing requires external text editing and post-processing consists of time series and contour plotting. Comparisons of model and field data must be done externally. The current version is not linked to GIS. The version under development will have GIS capabilities through ArcView.

Human Support

As developer and sponsor, HydroQual, Inc., provides user support and updates for the model. Workshops are offered, often annually, by HydroQual and/or Stevens Institute of Technology. No conferences or symposia were identified.

Model Usage

The list of ECOM / ECOMSED applications is extensive, numbering over 50 applications in the last 15 years. The current release of ECOMSED has a history of applications to oceanic, coastal and estuarine waters including Chesapeake Bay, New York Bight, Delaware River and Bay, the Gulf Stream Region, Massachusetts Bay, Georges Bank, Oregon Continental Shelf, New York Harbor, and Onondaga Lake.

Level of Effort – As is the case for all models in this evaluation, the level of effort depends on the application, but generally moderate to high.
Data Requirements – Moderate to high. Typical for this type of model and dependent on the application. Some interpretation may be required for generating input.
User Expertise - Moderate to high. Typical for this type of model and dependent on the application. Interpretation may be required for evaluating output.

### 3.3.4 EFDC

Overview

The Environmental Fluid Dynamics Code (EFDC) is an advanced three-dimensional, time-variable model that provides the capability of internally linking hydrodynamic, water quality and eutrophication, sediment transport and toxic chemical transport and fate sub-models in a unique single source code framework EFDC is designed to represent a finite difference computational grid as either a simple cartesian grid or an orthogonal, curvilinear coordinate system for irregular coastlines. In the vertical domain, EFDC uses a 'sigma-stretched-grid' to represent complex bathymetry. As a fully three-dimensional model, EFDC can be applied to all types of waterbodies. EFDC has been applied to over 100 waterbodies including the James River, Chesapeake Bay, Neuse estuary, the Indian River Lagoon, Peconic Bay (New York), Norwalk Harbor (Connecticut), the Housatonic River (Massachusetts), the wetlands of the Florida Everglades, the Blackstone River (Rhode Island), Christina River (Delaware), Schuykill River, Yazoo River and Wolf Lake (Mississippi), Ten Killer Reservoir (Oklahoma), Mobile Bay (Alabama) and Morro Bay (California).

Hydrodynamics

The hydrodynamic model of EFDC, comparable to the 'Blumberg-Mellor' ECOM /POM class of modern hydrodynamic model, accounts for all the major physical processes that govern the barotropic and baroclinic components of water motion in natural water systems. Prognostic state variables of EFDC include water temperature, salinity, water surface elevations and the 3D velocity/ flow field. Turbulent closure formulations are incorporated in the model to provide internal simulations of horizontal diffusion and vertical diffusion processes. The hydrodynamic model can be executed in two modes: (1) the results of the hydrodynamic model can be saved and used as input for the mass transport sub-models or (2) EFDC can be executed in a fully coupled mode with coupled simulations of hydrodynamics, sediment transport, toxic chemicals and eutrophication.

Sediment Transport

Similar to ECOMSED, the sediment transport model of EFDC incorporates advanced formulations based on the most recent research findings and understanding of sediment transport processes. EFDC internally computes settling, deposition and resuspension of cohesive and non-cohesive solids as well as sediment bed geomechanics. Water column and bed exchange of particles is represented as functional relationships of bed shear stress and bed shear strength for cohesive solids and the 'Shields' parameter for non-cohesive solids. Consolidation of the sediment bed is represented by a surface bed layer and multiple deep bed layers that respond to the accumulation or erosion of solids from the bed. Unlike ECOMSED, EFDC accounts for multiple classes of cohesive and non-cohesive solids and bedload processes. The sediment transport model of EFDC has been applied to Lake Okeechobee and Morro Bay.

Toxic Chemical Transport and Fate

The toxic chemical fate model incorporates detailed formulations for multiple chemicals similar to the formulations used in CE-QUAL-ICM/TOXI, RCA-TOX and WASP-TOXI. The contaminant fate model of EFDC accounts for multiple toxic chemicals and multiple classes of solids in an integrated model of hydrodynamics, sediment transport and toxic chemical fate. Sorbed contaminants are exchanged between the water column and sediment bed by deposition/resuspension and mixing within the bed. Dissolved contaminants are exchanged by porewater advection and diffusion within the bed and diffusion across the sediment-water interface. The sediment transport and contaminant fate models of EFDC have been applied for several contaminant fate studies including the Duwamish Waterway-Elliott Bay in Puget Sound, the Blackstone River (Rhode Island) and the Housatonic River (Massachusetts).

Conventional Pollutants and Eutrophication

The eutrophication model, functionally equivalent to CE-QUAL-ICM described above and RCA described in Section 3.1.2, is an advanced water quality model that directly links with the hydrodynamic model. The eutrophication model incorporates multiple functional groups of planktonic algae, dissolved oxygen, nutrient cycles of nitrogen, phosphorus and silica, organic carbon, chemical oxygen demand and total active metal as the 21 state variables of the model. Organic carbon and organic nutrients are represented as dissolved and particulate labile and refractory forms. The predictive sediment diagenesis model of Di Toro (2000) is incorporated in EFDC to internally couple the deposition of particulate organic carbon to the sediment bed with sediment-water fluxes of inorganic nutrients and dissolved oxygen. The eutrophication model of EFDC has been applied to several estuaries of the Chesapeake Bay system, Peconic Bay, the Christina River, Yazoo River and Wolf Lake, Mobile Bay and Ten Killer Reservoir.

Documentation

The documentation reviewed was "User's Manual for the Environmental Fluid Dynamics Computer Code" (Hamrick,1996). It consists of 185 pages. Other documents we reviewed are, "EFDC Technical Memorandum Theoretical and Computational Aspects of Sediment Transport in the EFDC Model, 2nd Draft" (Tetra Tech, Inc., 2000), 47 pages, and "A Three-Dimensional Hydrodynamic-Eutrophication Model (HEM-3D): Description of Water Quality and Sediment Process Submodels (EFDC Water Quality Model)" (Park et al., 2000).

The technical memorandum and revised water quality document extensively discuss theory. The coding structure is adequately presented in the three documents, and the FORTAN code is available.

The User's Manual's primary focus is the hydrodynamic model. There is a description of creating an output file for input into WASP5-EUTRO5. A separate report describes the eutrophication models incorporated into EFDC. At present there is no comprehensive user's manual that describes how to run the current version of the model with two built-in eutrophication schemes. It would be difficult for an inexperienced user to set up and run the model.

A version control scheme featuring software version numbers corresponding to specific documentation products appears to be absent from EFDC. Since EFDC has undergone continual enhancement, this omission complicates the process of understanding what model capabilities have been applied to what studies, and what code has been subjected to peer review at what point in time.

Application Aids

Windows graphical user interface is under development.

The pre-processor has a grid generator (GEFDC), an input data checker, and an initial condition generator. The post-processor converts output data for use by other third party visualization applications. Linkage to GIS is under development.

EFDC_Explorer, developed by Dynamic Solutions, is a Windows-based graphical user interface designed as a pre- and post-processor for EFDC. EFDC_Explorer has recently been licensed to EPA as a public domain tool to facilitate applications of EFDC for TMDLs and other modeling studies. The current version of EFDC_Explorer is designed to process data for the hydrodynamic and sediment transport models of EFDC.

Human Support

Model support by Tetra Tech is available on a cost reimbursement basis. An informal users group exists primarily to share experience and report potential code bugs and hardware/software incompatibilities. A web site is under construction. The SMIC website maintains a bulletin board for users of this model.

Conferences, Workshops, and Symposia - None identified.

Model Usage

The model has been used for discharge dilution studies in the Potomac, James and York Rivers. Salinity intrusion studies include the York River, Indian River Lagoon and Lake Worth. Sediment transport studies include the Blackstone River, James River, Lake Okeechobee, Mobile Bay, Morro Bay, San Francisco Bay, Elliott Bay, Duwamish River and Stephens Passage. Power plant cooling studies include Conowingo Reservoir, the James River and Nan Wan Bay. Contaminant transport and fate studies include the Blackstone and Housatonic Rivers, James River, San Francisco Bay, Elliott Bay and the Duwamish River. Water quality eutrophication studies include Norwalk Harbor, Peconic Bay, the Christina River Basin, the Neuse River, Mobile Bay, the Yazoo River Basin, Arroyo Colorado, Armand Bayou, Tenkiller Reservoir, and South Puget Sound. The Peconic Bay water quality application is particularly noteworthy. The model was calibrated using one year data set and subsequently validated by simulation of an eight year historical period having extensive field data. The model was then executed for 10 year management scenarios to develop a Comprehensive Conservation and Management Plan for the estuary system.

Level of Effort - High. The availability of pre- and post-processors reduces the effort involved in the construction of input data files and analysis of results.
Data Requirements **-** High
User Expertise **-** High in hydrodynamics, sediment and water quality chemical and biological interactions.

### 3.3.5 EFDC1D (Version 1.0)

Overview

EFDC-1D is a modified version of EFDC developed by Tetra Tech, Inc. for EPA Region IV to provide an advanced hydrodynamic and sediment transport model that can be applied for water quality simulations in branched networks of one-dimensional, variable cross-section streams and rivers. The results of the hydrodynamic and sediment transport model simulations can be linked as input to WASP5 and WASP6 for water quality evaluations for TMDLs and other water quality management planning purposes. The hydrodynamic, sediment transport, toxic chemical fate and eutrophication models of EFDC-1D are identical to the models available in EFDC. The descriptions of these sub-models will not be repeated.

Documentation

The documentation reviewed is titled, "EFDC1D, A One Dimensional Hydrodynamic and Sediment Transport Model for River and Stream Networks, Model Theory and Users Guide", May 2001 – 2nd Draft (Tetra Tech, Inc., 2001). It consists of 102 pages. The theory discussion is mostly on sediment and erosion. The model coding structure is not presented. Further improvements are not in progress at this time.

Application Aids

A graphical user interface, pre- and post-processors were not identified. The model requires text input, and generates text output. The ability to perform field-data model-data comparisons was not identified, but it is likely to be done externally to the model.

Linkage to GIS was not identified, but it is probably similar to the EFDC model.

Human Support

Similar to EFDC model

Model Usage

Two sample application file sets are provided with the EFDC1D model. The Los Angeles River network is relatively simple, with a main stem and seven second order tributaries. The Brandywine Creek, Pennsylvania and Delaware, consists of several branched segments separated by several dams.

Level of Effort – (Assumed similar to EFDC)
Data Requirements - (Assumed similar to EFDC)
User Expertise - (Assumed similar to EFDC)

### 3.3.6 HSCTM-2D (Version 1.0)

Overview

The Hydrodynamic, Sediment, and Contaminant Transport Model- 2 Dimensions model (HSCTM-2D) is a finite element modeling system for simulating two-dimensional, vertically-well mixed, surface water flow (typically riverine or estuarine hydrodynamics), sediment transport, and contaminant transport (Hayter et al., 1998). The modeling system consists of two modules: (1) the hydrodynamic model (HYDRO2D) and (2) the sediment and contaminant transport modeling (CS2D). HYDRO2D solves the equations of fluid motion while CS2D solves the advection-dispersion equation for nodal vertically-integrated concentrations of salinity, suspended sediment, dissolved and sorbed contaminants, and bed surface elevations. HSCTM-2D may be used to simulate both short term (less than 1 year) and long term scour and/or sedimentation rates, and contaminant transport and fate in vertically well-mixed bodies of water. HSCTM-2D has been applied to the Maurice River and Union Lake in New Jersey (Hayter and Gu, 1998) and a coastal marina sedimentation study (Smith, 1994).

Hydrodynamics

HYDRO2D solves the equations of motion and continuity for nodal depth-averaged horizontal velocity components and flow depths. The effects of bottom, internal and surface shear stresses, horizontal salinity gradients, and the Coriolis 'force' are represented in the equations of motion. HSCTM-2D can be run in an uncoupled or semi-coupled mode. In the uncoupled mode, HYDRO2D is run separately from CS2D. In the semi-coupled mode, HYDRO2D and CS2D are run as follows: HYDRO2D first calculates the flow field for the current time step; the predicted flow field is then used in CS2D to calculate the transport of sediments and contaminants during the same time step. HYDRO2D is run at every time step to update the flow field to account for predicted changes in nodal flow depths due to erosion and deposition.

Sediment Transport

HSCTM-2D is designed to represent processes that govern the transport of multiple classes of cohesive solids. Non-cohesive solids are not represented in HSCTM-2D. The model accounts for the mass transport of cohesive particles by advection and dispersion, aggregation, erosion and deposition. A layered sediment bed model is used in simulating bed formation and subsequent erosion of solids. Sediment bed structure (density and shear strength profiles, thickness and elevation), net change in bed elevation and net vertical mass flux of sediment over an interval of time (e.g., over a certain number of tidal cycles), average amount of time sediment particles are in suspension, and the downward flux of cohesive solids onto the bed are simulated for each finite element in the model domain.

Toxic Chemical Transport and Fate

HSCTM-2D simulates the adsorption and desorption of multiple classes of heavy metals with cohesive solids. HSCTM-2D employs a '2-phase' partitition model where the user assigns an appropriate value for the distribution coefficient ("Kd') to compute the dissolved and sorbed fractions of the heavy metal.

Conventional Pollutants and Eutrophication

HSCTM-2D does not include an internal eutrophication model. Organic carbon is not considered in the ‘2-phase’ partition model that is used to simulate the adsorption and desorption of heavy metals.

Documentation

The documentation for this model consists of “HSCTM-2D, A Finite Element Model for Depth-Averaged Hydrodynamics, Sediment and Contaminant Transport” (Hayter et al., 1998). It consists of 220 pages, with an extensive discussion of theory. The coding structure is presented with a flow chart, descriptions of subroutines, and a chapter titled, “Description of the Modeling Structure.” The FORTRAN source code is available.

Application Aids

Model documentation refers to “SMS” and “GFGEN” software for grid generation and output viewing. Input and output files are both text and binary formats. Post-processing with SMS produces vector plots, contours, and time history plots. Field data – model data comparison capabilities could be made using third party software external to the model. Linkage to GIS is not available.

Human Support

Support for this package comes from the EPA Center for Exposure Assessment Modeling website where the user can download the program, manual, and release notes for Version 1.01.

Workshops, user-oriented web sites, list server user groups, conferences and symposia were not identified.

Model Usage

HSCTM-2D has been applied to the Blackwater Branch, the Maurice River, and Union Lake near Vineland, NJ, by the model authors in order to understand the fate of arsenic contaminated sediments there.

Level of Effort - High. No pre- and post-processors increases the effort involved in the construction of data files and analysis of results.
Data Requirements - High. Suggests field measurements and lab testing of sediments for parameters used in model.
User Expertise - High

### 3.3.7 HSPF-RCHRES (Release 12)

Overview

Hydrological Simulation Program - FORTRAN (HSPF) is a comprehensive package for simulation of watershed hydrology and water quality for both conventional and toxic organic pollutants. HSPF incorporates watershed-scale models into a basin-scale analysis framework that includes fate and transport in one dimensional stream channels. It is the only comprehensive model of watershed hydrology and water quality that allows the integrated simulation of land and soil contaminant runoff processes with in-stream hydraulic and sediment-chemical interactions. The result of this simulation is a time history of the runoff flow rate, sediment load, and nutrient and pesticide concentrations, along with a time history of water quantity and quality at any point in a watershed. HSPF simulates three sediment types (sand, silt, and clay) in addition to a single organic chemical and transformation products of that chemical.

HSPF-RCHRES is used to route runoff and water quality constituents through stream channel networks and reservoirs. The module simulates the processes that occur in a series of open or closed channel reaches or a completely mixed lake. Flow is modeled as unidirectional. A number of processes can be modeled, including:

- Hydraulic behavior
- Heat balance processes that determine water temperature
- Inorganic sediment deposition, scour, and transport by particle size
- Chemical partitioning, hydrolysis, volatilization, oxidation, biodegradation, and generalized first-order (e.g. radionuclides) decay, parent chemical/metabolite transformations
- DO and BOD balances
- Inorganic nitrogen and phosphorous balances
- Plankton populations
- pH, carbon dioxide, total inorganic carbon, and alkalinity

<u>Hydrodynamics</u>

HSPF includes an internal one-dimensional hydrodynamic model based on the kinematic wave model. Hydraulic data is provided externally by the modeler as input data (‘F-Table’) to assign surface elevation and/or depth, surface area, cross-sectional area and volume for the network of river reaches assigned to represent the watershed.

<u>Sediment Transport</u>

The approach taken by the HSPF sediment transport code (SEDTRN) to compute transport of channel sediment is based on the SERATRA model developed by Battelle Laboratories (Onishi and Wise, 1979). Both noncohesive (sand) and cohesive (silt, clay) sediments are simulated in SEDTRN; migration of each sediment fraction between suspension in water and the bed is modeled by balancing deposition and scour computations. The code allows the modeler to compute the deposition or scour of noncohesive sediment by selecting one of three empirical formulations:

- A user-defined power function of streamflow velocity,
- A relationship (Toffaleti method) dependent upon median sand particle diameter, average stream velocity, reach hydraulic radius, reach slope, settling velocity for sand (user-specified), and water temperature,or
- A relationship (Colby method) dependent upon median sand particle diameter, average stream velocity, reach hydraulic radius, fine sediment load concentration, and water

temperature.

The simulation of cohesive sediment transport consists of two steps. First, advective transport is calculated; then deposition and scour is calculated based on the calculated bed shear stress. To evaluate deposition, the modeler is required to provide values for settling velocity and critical shear stress for deposition for each fraction (silt, clay) of cohesive sediment that is modeled. To evaluate resuspension, or scour, the modeler must provide values for the erodibility coefficient and critical shear stress for scour for each fraction. Ziegler and Owen (2001) have modified the sediment transport model of HSPF-RCHRES to include an option for selection of the more sophisticated sediment transport formulations used in ECOMSED and SEDZL (Ziegler and Lick, 1986).

Toxic Chemical Transport and Fate

The focus of the HSPF toxic chemical transport and fate code development was to allow simulation of agricultural pesticides and other synthetic organic chemicals. Given the diversity of pesticides that might be modeled, the code provides the user with the capability to model any subset of the following generalized processes: advection of dissolved material; decay of dissolved material by hydrolysis, oxidation by free radical oxygen, photolysis, volatilization, biodegradation, and/or generalized first-order decay; production of one modeled constituent as a result of decay of another constituent; advection of adsorbed suspended material; deposition and scour of adsorbed material; and adsorption/desorption between dissolved and sediment-associated phases. Using the toxic chemical transport and fate code (GQUAL) in conjunction with the sediment transport code (SEDTRN), adsorbed chemicals may settle or resuspend during each simulation time step, depending on hydrodynamic conditions. Decomposition of adsorbed chemicals may be simulated, both in suspended materials and in the bed, by using a first-order, temperature-corrected decay formulation.

Conventional Pollutants and Eutrophication

The HSPF code for Conventional pollutants and eutrophication (RQUAL) provides detailed simulation of constituents involved in biochemical transformations. Included are dissolved oxygen, BOD, ammonia, nitrite, nitrate, phosphate, phytoplankton, benthic algae, zooplankton, refractory organics, and pH. The primary dissolved oxygen and biochemical oxygen demand balances are simulated with provisions for decay, settling, benthal sinks and sources, reaeration, and sinks and sources related to plankton. The primary nitrogen balance is modeled as sequential reactions from ammonia through nitrate. Ammonia volatilization, ammonification, denitrification, and ammonium adsorption/desorption interactions with suspended sediment fractions are also considered. Both ammonium and phosphate adsorption/desorption to suspended sediment fractions are modeled using an equilibrium, linear isotherm approach. Both nitrogen and phosphorus species are considered in modeling three types of plankton - phytoplankton, attached algae and zooplankton. Phytoplankton processes that are modeled include growth, respiration, sinking, zooplankton predation, and death; zooplankton processes include growth, respiration and death; and benthic algae processes modeled are growth, respiration and death. Hydrogen ion activity (pH) can be calculated by two independent code sections. The first, named PHCARB, is contained within the RQUAL section and computes pH by considering carbon dioxide, total organic carbon and alkalinity. In doing so, the code considers the effects on the carbon dioxide-bicarbonate system of carbon dioxide invasion, zooplankton respiration, BOD decay, net growth of algae, and benthal releases.

Documentation

The HSPF RCHRES user's manual is not a separate document but is incorporated into the 873 pages of the HSPF user's manual which is maintained and updated by the USEPA ERD in cooperation with the USGS Office of Surface Water. The Version 11 documentation is distributed with the model, and is dated 1996. The manual is technically very well written with a wealth of information, but it would be difficult for the inexperienced user to construct a data set and use the model.

The user's manual, Release 12 is available from EPA OST in support of BASINS application. The documentation is clear and complete; however, due to the complexity of the model it is not exhaustive. Problems can be encountered in model applications that are not addressed by the available documents. Most of these problems can be resolved by submitting questions to the list server. "Hydrological Simulation Program -- FORTRAN User's Manual for Release 12" (Bicknell et al., 2001) is divided into 3 major sections: theory, table structure and parameter definition, and time series attributes and requirements. An independent program built around a Microsoft Access database describes some statistical attributes of most of the available model parameters. The program is called HSPFParm (Donigian et al., 1999).

An Expert System has been developed for calibration of the hydrology component of HSPF. This program is called HSPEXP and is available from the USGS. Documentation for this program is not extensive but is valuable to model application even if the HSPEXP program is not used. See Lumb et al., 1994. An application guide (Donigian et al., 1984) is available that provides suggestions on the appropriate application strategy for the model.

The FORTRAN code is public domain, modular, and well documented. Programmers can generally follow the code easy enough, although, problems can arise due to the sheer number of modules and linkages.

Application Aids

The post-processor of choice was GenScn (Kittle et al., 1998) which was implemented independently or through EPA's BASINS software. The graphical pre- and post-processor, GENSCN, is available from http://water.usgs.gov/software. HSPF-RCHRES is linked to GIS through BASINS and GenScn, and requires ArcView 3.2.

WIN-HSPF (Duda et al., 2001), with user's manual provides a graphical user interface. The pre-processor generates input files, and the post-processor allows viewing of available output files. The interface also handles model-field comparisons for most types of field data. The Windows version user's manual is a separate document.

Human Support

Support is provided to USGS offices and to agencies cooperating with the USGS on modeling studies. Limited support may be available to others. Contact can be made through h2osoft@usgs.gov.

EPA support for HSPF is coming from an IAG (interagency agreement) with the USACOE at WES. Support is primarily limited to state, local, and federal personnel.

Model distribution: http://www.epa.gov/ceampubl/swater/index.htm or
http://www.epa.gov/waterscience/basins.htm or
http://water.usgs.gov/software/hspf.html

There is an active list server for HSPF. Instructions for joining are located at: http://www.eos.uoguelph.ca/webfiles/james/homepage/Research/ListServers.html

HSPF RCHRES users can also contact other users at the EPA-sponsored BASINS list server at: http://www.epa.gov/ost/BASINS/

Conferences, Workshops, and Symposia were not identified. There are, however, periodic EPA-sponsored HSPF training workshops.

Model Usage

HSPF applications since its inception in 1980 have been worldwide and number in the hundreds; nearly all HSPF applications have included application of both the landscape (PERLND, IMPLND) modules and the receiving water (RCHRES) module. While numerous HSPF applications have been focused on evaluating 'hydrology-only' issues, dozens of applications have focused on sediment transport, nutrient cycling, pesticide fate and transport and related water quality issues. The model has been applied to such diverse climatic regimes as the tropical rain forests of the Caribbean, arid conditions of Saudi Arabia and the Southwestern U.S., the humid Eastern U.S. and Europe, and snow covered regions of Eastern Canada.

Level of Effort – Moderate to High. The availability of pre- and post-processors reduces the effort involved in the construction of data files and analysis of results.
Data Requirements –Moderate to High. HSPF RCHRES is an 1-dimensional model, but requires input for 15 state variables.
User Expertise – Moderate to High. The eutrophication model uses 15 state variables. The user needs to define forcing functions and parameters, to understand model set-up and linkages. The model requires a large quantity of data; e.g. GIS, weather, land use, physical descriptors, water quality constituents, calibration data.

### 3.3.8 IPX (Version 2.7.4)

Overview

The In-Place Pollutant Export Model (IPX) has been developed as a 'cousin', or variant, of WASP4-TOXI (Ambrose et al., 1988) in support of the Lake Michigan Mass Balance Study. IPX has been applied for an assessment of sediment transport and PCB fate in the Lower Fox River and Green Bay (Velleux et al., 2001).

Hydrodynamics

As a 'cousin' of WASP-TOXI, IPX does not include an internal hydrodynamic model. Transport data is externally provided to IPX either as a (a) flow balance and flow routing defined by the modeler; or by (b) linkage of the results generated by a separate hydrodynamic model. In the Lower Fox River and Green Bay application, ECOM-3D was applied to provide hydrodynamic input to IPX.

Sediment Transport

As a WASP 'cousin', IPX represents three generalized size classes of solids as state variables of the sediment transport sub-model. IPX Version 2.7.4 synthesizes sediment transport processes for sediment aging, decreased sediment resuspendability with increasing age and resuspension of fresh deposits of sediments as functions of water velocity (bottom shear stress). Using a 'Lagrangian' approach to track the accumulation and erosion of sediments in the bed, IPX Version 2.7.4 incorporates a very different methodology than the 'Eulerian' approach used by WASP to represent sediment bed consolidation and erosion. These processes were incorporated to realistically represent toxicant transport and fate and significantly improve the model framework for application to tributary systems subject to significant deposition and erosion.

Toxic Chemical Transport and Fate

Unlike the limitation imposed by WASP-TOXI where no more than three toxicants can be simulated in a model run, IPX Version 2.7.4 allows for the simulation of any number of chemicals simultaneously within a single model run. In addition to hydrolysis, photolysis, volatilization, oxidation, and biodegradation as loss processes, chemical fate processes in IPX include equilibrium partitioning with the organic carbon fraction of solids.
Unlike WASP-TOXI, IPX does not allow for simulation of ionic speciation.

Conventional Pollutants and Eutrophication

IPX does not include conventional pollutants and eutrophication. The organic carbon fraction of organic matter is assigned as a user-defined empirical forcing function for input to the toxic chemical model.

Documentation

The documentation reviewed is titled "A User's Guide to IPX, the In-Place Pollutant Export Water Quality Modeling Framework", Version 2.7.4 (Velleux et al., 2000). The EPA version of the same name is dated November 2001. The document is 195 pages long. It contains an extensive discussion of theory, 86 pages. The coding structure is presented in flowcharts and subroutine descriptions. Portions of IPX Manual (Model Theory, Input Data Structure, and Programmers Guide) are derived from WASP4 and WASP5.

Application Aids

IPX has no graphical user interface. Text-based FORTRAN programs are available for some pre- and post-processing. The pre-processor can read USGS stream flow files for input to the model. Post-processing with the program W4DIS (W4DIS274) reads binary output files and pulls out parameters selected by the user. Third party software is required for graphics and comparisons to observed field data. Linkage to GIS is not available.

A DOS-based pre-processor program is available from Dynamic Solutions to generate the input files needed to execute IPX Version 2.7.4. The IPX preprocessor, adapted from the WASP5 preprocessor developed for Version 2.0 of EPA's National Water Pollution Control Assessment Model (NWPCAM) (Bondelid et al., 2001), is designed to model either a single river reach or a branched network of river reaches. River reaches are organized at the Rf1 and Rf3 levels by the hydrologic catalog units of the 18 major river basins of the conterminous United States. The IPX pre-processor allows the flexibility to specify either a 1D(x) or 2D(x,z) spatial domain as: (a) single, or multiple, water column layers; and (b) zero, single or multiple sediment bed layers. A WASP5 post-processor program, adapted to post-process the results generated by IPX, displays model results as: (a) time series [C(t)]; (b) spatial transects [C(x)]; or (c) depth profiles [C(z)]. Plots are generated as Hewlett-Packard Graphic Language (HPGL) plots using PRINTGL.

<u>Human Support</u>

The developer, Mark Velleux, is currently attending graduate school. Support available for model application is uncertain.

<u>Model Usage</u>

IPX was initially developed during a comprehensive analysis of the Lower Fox River, WI to predict future loadings into Green Bay, WI. Subsequently, IPX was applied to the Buffalo and Oswego Rivers in New York. IPX Version 2.7.4 was the result of a collaborative effort between the USEPA Large Lakes Research Station and the Wisconsin Department of Natural Resources.

Level of Effort - Moderate to High. Requires external construction of input data files and analysis of results. As is the case for all models in this evaluation, the level of effort depends on the application.
Data Requirements - Moderate to High. Typical for this type of model and dependent on the application. Interpretation is required for generating input.
User Expertise - Moderate to High. Similar to WASP.

### 3.3.9 WASP5 (Versions 5.10 & 6.0)

<u>Overview</u>

The Water Quality Analysis Simulation Program (WASP) is a general purpose water quality model developed to simulate the transport and fate of conventional pollutants and toxic chemicals in natural water systems. WASP5, Version 5.10, was released as a DOS-based program in 1993 by EPA Center's for Exposure Assessment Modeling in Athens, Georgia (Ambrose et al., 1993). A GUI-based Windows version of WASP (WASP6, Version 6.0) was released by EPA Region IV in March 2001 (Wool et al., undated). A Windows-based preprocessor is incorporated directly into the WASP6 model structure. Unlike the DOS-based WASP5 model, separate pre-processor and post-processor programs are not required to use WASP6.

WASP represents time dependent advection and dispersion within a generalized multi-dimensional framework [1D(x); 1D(z); 2D(xy); 2D(xz); 3D(xy,z)] that can be used to represent processes and interactions within a surface and subsurface water column. Surface and subsurface layers of a sediment bed can also be defined to simulate exchange processes between the water column and the sediment bed. The finite difference, explicit numerical integration methods of WASP are based on solution techniques presented in Thomann and Mueller (1987). WASP is designed with the following three main components: (1) mass transport by advection and dispersion; (2) point and non-point source pollutant loads and (3) kinetic processes and interactions. The kinetics component of WASP is developed as two separate sets of code for: (1) dissolved oxygen, CBOD, nutrients and eutrophication (EUTRO); and (2) sediment transport and toxic chemicals fate (TOXI). WASP is unique in it's flexibility to allow the development of 1D, 2D or 3D models driven by either steady-state or time-variable flows, pollutant loads, external forcing functions and boundary conditions. WASP is also unique in that once a computational domain is defined to represent the model segments, flow balances, transport routing and specification of boundary conditions and pollutant loads, the data can be used for both the eutrophication model (EUTRO) and the toxic chemicals model (TOXI). WASP is a well-established model with a proven track record of many water quality analyses of dissolved oxygen, nutrients, eutrophication and toxic chemicals in all types of waterbodies (Lung, 2001; Martin and McCutcheon, 1999).

Hydrodynamics

WASP does not include an internal hydrodynamic model. Time-dependent hydraulic data is provided externally as input data to assign flow, velocity, water column depth, surface area, cross-sectional area and volume of each segment defined to represent the waterbody. Transport data is externally provided to WASP either as (a) flow balance and flow routing defined by the modeler; or by (b) linkage of the results generated by a separate hydrodynamic model. The hydrodynamic results from EFDC and EFDC-1D, for example, can be linked as a file for input to WASP5 and WASP6.

Sediment Transport

Suspended solids and sediment bed solids are incorporated in WASP-TOXI with the capability to represent three generalized size classes of solids as state variables. WASP-TOXI does not include an internal sediment transport model. Time-dependent and spatially-dependent velocities are assigned as input data to define settling, deposition, resuspension and deep burial rates of solids. At a minimum, a spatial characterization of the solids concentration in the surficial sediment bed is needed for the simulation of resuspension conditions. WASP also includes the capability of describing multiple sediment bed layers using a simplified representation of bed consolidation and erosion. Advanced sediment transport models, such as SEDZL, have been linked with WASP-TOXI to provide the required water column-sediment bed deposition and erosion fluxes of solids. Analysis of site-specific field data has also been used to determine particle settling, deposition, resuspension and deep burial velocities for input to WASP-TOXI. To overcome the limitations of WASP that are imposed by the need to externally assign deposition and resuspension velocities, a modified version of WASP5-TOXI has been developed by the Interstate Commission on the Potomac River Basin. This modified version of WASP5-TOXI incorporates the sediment transport formulations used in HSPF-RCHRES to provide an internal simulation for the sediment transport model of WASP5-TOXI (Mandel and Schultz, 2000).

Toxic Chemical Transport and Fate

WASP-TOXI is designed to provide simulations of the transport pathways and fate for three toxic chemicals and three suspended solids classes in the water column and sediment bed. In addition to hydrolysis, photolysis, volatilization, oxidation, and biodegradation as loss processes, chemical fate processes in WASP-TOXI include equilibrium partitioning with the organic carbon fraction of solids.

Conventional Pollutants and Eutrophication

WASP-EUTRO provides the capability to simulate dissolved oxygen, CBOD, nutrients and algae with 8 state variables in an intermediate level model. Organic matter is represented as carbon (as CBOD), organic nitrogen and organic phosphorus. Dissolved and particulate fractions of these state variables are empirically assigned using spatially-dependent data. Labile and refractory decomposition rates are combined as a 'lumped' decay rate for organic matter. Planktonic algae are represented as a single 'lumped' assemblage of algae; WASP-EUTRO thus does not have the capability to represent seasonal succession of algae species groups. WASP5-EUTRO (Version 5.10) does not include coliform bacteria as a state variable. WASP6 does include a new set of kinetic routines designed to simulate water temperature and coliform bacteria. Research Triangle Institute (RTI) has integrated a modified version of WASP5-EUTRO (Version 5.10) into the National Water Pollution Control Assessment Model (Bondelid et al., 2001). The three additional state variables included in the RTI modified version of WASP5-EUTRO are inorganic suspended solids, salt (as salinity, chlorides, total dissolved solids or specific conductance), and total and/or fecal coliform bacteria.

Sediment-water exchange of nutrients and dissolved oxygen is included in WASP-EUTRO using two optional approaches: (1) externally defined empirical forcing functions for benthic nutrient regeneration rates and sediment oxygen demand; or (2) internally simulated sediment-water exchange of nutrients and dissolved oxygen using a diffusive flux methodology developed for Lake Erie (Di Toro and Connolly, 1980). To improve the capability of the benthic exchange approach, Lung (2001) has incorporated Di Toro's (2000) advanced sediment diagenesis model in a modified version of WASP5-EUTRO developed for an application to the Anacostia River in Washington DC (Mandel and Schultz, 2000).

Documentation

The documentation that was reviewed is "Water Quality Analysis Simulation Program (WASP), Version 6.0, Draft: User's Manual" (Wool et al., no date). It is clear and complete, consisting of 267 pages. It provides an extensive discussion of theory. The model coding structure is presented, and the FORTRAN source code is available.

"The Water Quality Analysis Simulation Program, WASP5, Part A: Model Documentation" (Ambrose et al., 1995) was also reviewed. It consists of 251 pages. The new WASP6 manual is more extensive than earlier versions. The WASP5-EUTRO5 user's manual is maintained and updated with the model by the USEPA ERD. The version distributed with the model is dated 1993. Part B of the 1995 manual "The WASP5 Input Data Set" occasionally refers to EUTRO4 and perhaps needs an editing update. The manual would allow an inexperienced user to set up and run the model.

Application Aids

Version 6, WASP6, comes with a graphical user's interface described in the Version 6 user's manual. Pre- and post-processors are available. Linkage to GIS is available through ArcView, which must be purchased separately.

Version 5 has a DOS based pre-processor which generates data sets for DYNHYD5 and WASP5 and a DOS based post-processor for producing tables and graphs of model output.

In addition to the pre-processor provided by EPA CEAM in Athens, GA, an alternative DOS-based WASP5 pre-processor program is available from Dynamic Solutions to generate the input files needed to execute WASP5-EUTRO5 and WASP5-TOXI5. This WASP5 preprocessor has been developed as a component of Version 2.0 of EPA's National Water Pollution Control Assessment Model (NWPCAM) (Bondelid et al., 2001). The pre-processor is designed to model either a single river reach or a branched network of river reaches. River reaches are organized at the Rf1 and Rf3 levels by the hydrologic catalog units of the 18 major river basins of the conterminous United States. The WASP5 pre-processor is designed to define the WASP5 segment grids as a laterally-averaged water body or a branched network of tributaries in a watershed. along the longitudinal (x) and vertical (z) dimensions. The pre-processor allows the flexibility to specify either a 1D(x) or 2D(x,z) spatial domain as: (a) single, or multiple, water column layers; and (b) zero, single or multiple sediment bed layers. A WASP5 post-processor program has also been developed to facilitate the extraction of the WASP5 simulation results to display model results as: (a) time series [C(t)]; (b) spatial transects [C(x)]; or (c) depth profiles [C(z)]. Plots are generated as Hewlett-Packard Graphic Language (HPGL) plots using PRINTGL.

Human Support

Developer/Sponsor and Third Party Support – None identified.

User's Groups - None identified.
Model Distribution:
http://smig.usgs.gov/smic/
http://www.epa.gov/waterscience/wqm/

There is an active list server for WASP5. Instructions for joining are located at:
http://www.eos.uoguelph.ca/webfiles/james/homepage/Research/ListServers.html

Conferences, Workshops, and Symposia - None identified.

Training workshops are available for the newer WASP6 version.

Model Usage

Multiple versions of WASP have been used for over 20 years in a wide range of regulatory and water quality management applications for rivers, lakes, and estuaries. It has been used to examine eutrophication and PCB pollution of the Great Lakes, eutrophication of the Potomac Estuary, kepone pollution of the James River Estuary, and the transport and fate of organic contaminants in Lake St. Clair, Michigan. Other applications have been to simulate the transport and fate of DO, BOD, and organic nitrogen in untreated wastewater discharges, and to characterize the impact of agricultural activities on instream water quality in a periphyton dominated stream. EUTRO5 has been used in a full three-dimensional application in conjunction with the EFDC hydrodynamic model to assess the effectiveness of options for total nitrogen removal from a wastewater treatment plant.

Level of Effort - Moderate. The availability of pre- and post-processors reduces the effort involved in the construction of input data files and analysis of results.
Data Requirements **-** Moderate. Depends on the use of WASP as a 1-, 2-, or 3-D model.
User Expertise **-** Moderate. The eutrophication model uses only 8 state variables but it contains the option to activate a simplified benthic flux model to compute sediment oxygen demand and inorganic nutrient fluxes.

### 3.4 Model Linkage Issues and Strategies

Until the advent of watershed-scale assessments, and more recently TMDLs, regulatory and management concern with the quality of receiving waters had usually been addressed with "receiving waters only" models. However, estimation of pollutant loads from the source watershed is a necessary input for these models as a boundary condition; traditionally, these boundary conditions were often estimated very simply as constant, or monthly variable, loads using simple spreadsheets and assumptions. A watershed model that is calibrated to the available data and provides load estimates at the necessary time and space scales offers the most useful and reliable source of the information needed by the waterbody model. Furthermore, watershed models become mandatory when the problem definition requires explicit consideration of nonpoint sources and the impact of land-based Best Management Practices, such as needed for TMDLs.

While waterbody models have a strong need for watershed models, comprehensive watershed models also have needed to incorporate more detail in how they model the waterbody components of a watershed. For example, HSPF could be used to model the entire watershed including its waterbodies, but lakes and reservoirs that exhibit significant longitudinal and vertical water quality gradients are not well represented by the fully-mixed assumption made for an HSPF-RCHRES reach. The needs of comprehensive watershed water quality analyses are best met when the waterbody and the watershed models are linked to combine their respective strengths and capabilities.

Watershed models produce output for the following quantities, at time scales that vary with the specific watershed conditions and the specific model being applied. Waterbody models need many of these same quantities as inputs:

- Water inflow rate at waterbody boundaries,
- Boundary load or concentration of sediment in different size fractions,
- Boundary load or concentration of contaminants adsorbed to solids and in solution form,
- Boundary load or concentration of inorganic nutrients and organic matter in particulate and dissolved forms

Though the input and output are complementary, coupling requires attention to at least the following:

- Unit and dimension conversions, e.g., runoff in inches needs to be converted to a volumetric flow rate for input to a waterbody model

- Speciation or aggregation of constituents, e.g., partitioning of organic matter into labile and refractory fractions
- Interpretation and/or transformation of each constituent that is linked across the two models, e.g., does “phosphorus” refer to total P or only inorganic P? This issue is important because watershed and waterbody models may differ in the process coefficients and formulations.

Coupling of the watershed and waterbody models can be a loose coupling (e.g., EPA Chesapeake Bay nutrient study) where the models are essentially run independently of each other and files are exchanged between them through user manipulation of interface programs. Such a coupling is easy for the programmer and most flexible to model modifications, but most demanding of user time and attention to detail. At the other extreme, the coupling can be a tight coupling where the code for the two models is integrated into a single entity. Such a coupling is very inflexible, most demanding of the programmer’s time and attention to detail, but easy to use for the less experienced modeler; in addition, a tight coupling is generally computationally more efficient. The ideal watershed-waterbody coupling for an application will generally be some intermediate solution that reflects various application-specific factors.

This discussion addresses the final objective of this study: an evaluation of issues and strategies involved in linkage of selected waterbody model(s) to a comprehensive watershed model (see Section 1.2.1). The results of this effort are expected to serve as a starting point for a watershed-waterbody model integration effort. We refer to such an integrated system as the "watershed-waterbody modeling system" (WWMS).

Previous sections in this report have recognized four components that are included in developing a complete receiving water modeling capability. These four components are: hydrodynamic, sediment fate and transport, toxicant fate and transport, and conventional pollutants fate and transport. The models reviewed in earlier sections of the report are distinguished from the generic use of the term “model” in this discussion by referring to them as “named models”.

In many cases waterbody models need to have all four components before being applied to a problem. Thus, implicit in the linkage of a receiving water model with a watershed model is the integration of one or more named models to complete a waterbody model with the full complement of all four modeling components. With the exception of EFDC, the named models included in this review do not include all four components. The linkage issue is thus best addressed as a linkage of all four components as well as the watershed model. The watershed-waterbody linkage investigation then becomes an investigation of custom configurations that design and implement as many interfaces as the information-transfers required among the four components and one or more watershed model components. Examples of this approach are coupling an estuary model with HSPF (Donigian et al., 1998), linkage of a proprietary 3-D model with HSPF (Kolluru, 2003) and a coupling of GWLF with CE-QUAL-W2 (Jain, 2001). However, the possibility of multiple custom configurations complicates broad-based reviews such as this, because it is possible to mix and match the named models in different configurations. There would be an excessive number of combinations that needed to be reviewed if all named models were reviewed for compatibility in all configurations.

This implication, combined with prior Study Team experience with inter-model linkages through several model application life cycles, led to a further simplification as well as generalization. The discussion that follows is built around the concept of a generic information exchange structure. In such an architecture, each named model would query or provide information to this structure in a standardized manner. The design, implementation (and possibly performance) overheads in such a system would be small relative to the savings accruing from the operational and conceptual simplicity of this design in all new applications. Using a modular and generic design would also reduce the effort required to maintain complex watershed-waterbody model applications against user, modeler, and programmer turnover. Finally, efforts towards developing such a generic system would likely lead to convergence of future model and model version architectures, at least in their input/output relationships, and perhaps in their internal coding structures as well.

For purposes of this review it is sufficient to think of the information atom in such an information exchange structure to be a "dataset" and not discuss further any implementation or conceptual issues related to implementation of such a structure. This does not leave the concept as an unusable abstraction; as such implementations already exist within the context of surface water models. Watershed Data Management (WDM) files implement timeseries, table, and spatial datasets. WDM files have been well tested over time with regards to the adequacy of their conceptual basis, and have been used to implement model linkages among HSPF, SWMM, MODFLOW, AQUATOX, and others. Equivalent definitions can also be implemented in more modern web-enabled architectures using XML schemas.

In this review, we first identify various issues involved in watershed-waterbody linkage. This discussion is used to develop criteria that are used to evaluate individual named models. A preliminary narrative evaluation follows and is summarized in an evaluation matrix. The depth to which each named model was reviewed had to be limited, but the discussion and development of the linkage problem that is presented here will serve as an excellent starting point for strategic as well as tactical planning of a future watershed-waterbody model integration effort at EPA.

### 3.4.1 Watershed-Waterbody Model Linkage Issues

Linkage issues were identified by reviewing past combined watershed-waterbody modeling efforts and by anticipating issues that may occur in future integration efforts. Some issues were largely conceptual in nature and some were predominantly an issue of implementation, but usually there was a conceptual as well as an implementation aspect to linkage considerations.

Time scale matching is frequently cited as a concern in model linkage. It is generally desirable for the information source (usually a watershed model) to be finer in scale than the information sink (usually a waterbody model). However, in many, if not most, situations, the opposite occurs: watershed models are often run at daily timesteps, with the most detailed models, like HSPF, using timesteps in the range of one hour, or down to 5 or 15 minutes, for small urban watersheds. On the other hand, hydrodynamic waterbody models often run on timesteps of minutes or seconds, creating a situation where the watershed model inputs must be disaggregated in time. Environmental models require a large number of poorly characterized inputs, and a rigorous enforcement of a hierarchy of time scales in information moving from model to model is not practical. Time scale matching must often be addressed on a case-by-case basis, considering the specific watershed and waterbody conditions and the specific models involved.

Process formulation incompatibility among models that may be considered for linkage can be problematic. For example, a model may skip the carbonate equilibrium computations considering them irrelevant to lake phytoplankton dynamics, but another model may require alkalinity loadings for pH computations important to metal speciation. Organic matter needs to be partitioned into labile/refractory and dissolved/particulate when moving from the two watershed components in HSPF (IMPLND and PERLND) to the RCHRES module. In a similar fashion, sediment output for erosion contributions (from PERLND/IMPLND) needs to be partitioned into sand, silt, and clay for use in the RCHRES module.

Because of the complexities involved in characterization of organic matter, most models use slightly different "currencies" for this important water quality constituent. Conversions are often required for organic matter when moving from measurements to models and from one model to another. Such inter-conversions are best handled by making explicit the conversion method and assumptions being used. For example, a modeling study underway in King County, Washington is using an *average* organic matter composition as estimated from stream measurements for organic nitrogen, carbon and phosphorus and an assumed stoichiometric relationship. In a similar mapping from measurements to model variables other studies (Jain 2002, Jain et al., 2002) have used a stoichiometric relationship and the *minimum* of the measurements for organic nitrogen, carbon and phosphorus, and allocated the remainder of the measured nutrients to inorganic forms. The first approach will likely provide the best estimate of organic matter while the second approach preserves the nutrient budgets at the risk of producing unrealistic concentrations. If the WWMS were to use the elemental concentrations as the basis of exchange, it would standardize the information as well as force a documentation of the assumptions in each model participating in the exchange.

When conversions are done between seasonally variable quantities like chlorophyll and organic carbon, conversion factors for alternative algal stoichiometry can be implemented as a time series in the generic information exchange structure. The generic information exchange should be implemented at the highest possible level of detail. This would ensure a careful and explicit documentation of assumptions implicit in each model, and therefore in the model linkage. It would also ensure that models included or modified later in an application cycle would not require a retrofit to a model completed earlier in that application.

Model linkage requirements may also be dependent on the domain. For example, HSPF-RCHRES does not have tidal capability, so the watershed model HSPF requires linkage to an external waterbody model when the receiving waterbody is tidal, but not when it is riverine.

Operational issues involved in linkage are largely attributable to input and output file format issues. The file format issue would be automatically resolved if each named model in the WWMS is exchanging information with other models through a generic information exchange structure (e.g. WDM files). Filters specific to the named model can be written once and used for interfacing with all other models that have a useful degree of scientific compatibility with that model.

Another operational issue is the sometimes very large difference in run time between models. In an ideal linked model setup, the level of detail in each module will be matched to the overall problem's need for computational sophistication from that module. However, since modeling is frequently an exploratory exercise, this may be the endpoint rather than the starting point in any new model application.

Some other conceptual issues need to be addressed in development of a WWMS. Storage of material in a watershed model is frequently important to the predictions from a watershed model. The importance of initial conditions to a receiving waterbody model tends to be low for hydrodynamic components, but can be very high for sediment and contaminant components. Thus, in a WWMS the spin-up requirements for different components may be different. Other ways of matching of initial conditions between watershed and waterbody models may have to be investigated, e.g., by including initialization as one of the types of information exchange included in the generic information exchange.

Consideration was also given to whether there were any realistic needs for flow of information from waterbody modeling components to watershed components i.e. feedback between/among the linked models. An example of this may be seepage loss from the waterbody into watershed during drought periods or in arid watersheds, e.g. 'losing' and/or ephemeral streams. Other possible examples are: a waterbody exchanging water with a wetland, and large floodplain areas subject to wetting and drying. Such instances may be sufficiently rare or insignificant that they do not justify inclusion in a general WWMS, but the capability may be required in specific environmental settings. However, a unidirectional flow of information from watershed components to waterbody components is not a *requirement* in the proposed architecture; implementation of a bi-directional capability is doable. Inter-process communication between models can facilitate bi-directional flow of information between models. Since various waterbody model components generally serve as both input and output for each other among themselves anyway, assuming unidirectional information flow for waterbody models alone does not seem to offer any significant opportunity for simplification of the architecture. However, for linkage between watershed and waterbody models, at a process level, significant programming changes may be required to implement the appropriate feedback at each timestep, and may further require joint execution of both models in the linked mode.

Another conceptual issue is in the spatial detail and distribution of the load predicted from a watershed model. The watershed load could be a distributed load to the entire receiving stream length (as in HSPF), representing local direct inflows from adjacent land, or it could be a load at the watershed pour point (as in GWLF), represented as a 'pseudo' point source. Waterbody models may need to be analyzed to assess the potential impacts (and sensitivity) to alternate spatial distributions of input loads.

### 3.4.2 Evaluation Criteria

The issues discussed above were distilled into the following questions asked of each model for judging its compatibility with watershed models through a WWMS. The named models are not static entities, hence we focused on the potential compatibility of a named model, ignoring the straight-forward compatibility issues that could be addressed with a few days or hours of effort.

By proposing a generic information exchange structure that mediates all exchange of information, the compatibility issue is reduced from evaluation of a pair of models to evaluation of a single model. The highest scoring model would be one that is easiest to couple to the WWMS in an operational sense, and when so coupled, is compatible with the largest possible number of models in a conceptual sense. The first two criteria below address operational compatibility with the WWMS and the last three address conceptual compatibility.

Input/output Data Encapsulation

1) Is there a recognizable native data structure that encapsulates the inputs and outputs for the model? The data structure may be composed of more than one type of files, or a variable number of files. An example of a low scorer on this criterion is a model where much of the model information is embedded within the programs, or visible only as screens. Inputs and outputs being scattered across many files in a haphazard form, as generally occurs with a long history of ad hoc modifications by a large number of users, will lead to a low score on this criteria.

Code Encapsulation

2) Is the code to read and write from this data structure already available as subroutines or easily extractable into subroutines? Examples of low scorers on this question will be models that have input and output deeply embedded within and enmeshed with model logic. This criterion is not a strict requirement, however, because a named model that has a low modularity of input and output need not query the WWMS directly, but can instead work with the WWMS through a "wrapper", i.e. code that will mediate its interactions with WWMS. In practice, wrappers do impose limits on the types of interaction that can be supported.

Time and Space Resolution

3) We assumed a typical timescale for input and output of each module, elaborated in Table 3.11. How compatible is the named model's input and output with these WWMS time scales? Incompatibility may arise between models due to incompatible model formulations, but the WWMS should support several time scales for input and output of flows, loads and other supplemental information like time-varying conversion factors and forcing functions. Another source of incompatibility maybe a fixed and inappropriate time step embedded in the model implementation.

Table 3.11. Typical Time Scales of Functional Modules

| | Input | Output |
|---|---|---|
| Watershed | minutes to days | minutes to days |
| Hydrodynamic | minutes to hours | minutes to days |
| Sediment Fate & Transport | minutes to days | days to weeks |
| Toxic Chemical Fate & Transport | hours to years | hours to years |
| Conventional Pollutant Fate & Transport | hours to days | hours to days |

How is spatial resolution handled in the named model? Various components in a WWMS operate at different space scales. Space scales are usually not implied in a model's formulations and its programming as time scales sometimes are. Therefore the key question in this regard is how compatible is the module with multiple spatial compartments that may be defined in a WWMS. The spatial compartment definitions would need to be supported with individual properties like area, volume, depth as well as with inter-segment properties like "below", "downstream of", "adjacent to" to support inter-segment flux computations in a receiving water model.

Scientific Compatibility

4) The evaluation is not for compatibility between any two named models, but between the WWMS and the named model in its role as one of four functional components. Given that, the compatibility is highest for a model that has low input requirements and a large number of outputs. In that sense, this is a score of model generality. However, input and output detail generally go hand in hand in a well designed model, else there is either too little information going in or too little coming out. Therefore, the highest score will be for a model that has a selectable level of detail for inputs, outputs and internal computations. Such a hierarchical model can thus offer compatibility with a large number of models that depend on it for information, without being too restrictive of models it could use information from. This criterion is more appropriate for a pair of models than for a model by itself, as the WWMS is designed for being able to use models with differing degree of detail, while offering aggregation/disaggregation/conversion methods necessary to allow interaction with other models. Thus most models appeared to have a medium score on this criterion.

A narrative evaluation and qualitative scoring approach was favored over developing a quantitative system of assigning points for each model. The criteria can be made quantitative when a detailed specification for the WWMS is available. In fact, the rigorous assessment of a named model against such a specification is also a first step in integrating that model with the WWMS.

### 3.4.3 Narrative Evaluation of Named Models

Models identified in the screening process (Section 3.1.2) are discussed in alphabetical order below.

AQUATOX

The basic unit of the AQUATOX model is a "study". The study is entirely contained in a ".APS" file. The study contains site data, loads, parameter values, run start and end time, results, and may also contain values from a prior simulation. A study is a self-contained complete archival of all relevant values for regulatory purposes. Values used repeatedly can be saved in a library. The library is a PARADOX database that contains records for each site, organism or substance. This database will be ideal for interfacing with the "dataset" implementation chosen for the WWMS. It is not clear from the manual if the database library can also contain the results of a model run. In any case, the model results are exportable to txt, dBase, and Paradox formats. Paradox files are named with non-standard extensions (.SDB, .CDB, .PDB, and .ADB) in AQUATOX. Data splitting and merging across multiple files will be required. Two digit years are interpreted as 2000+ two-digit year regardless of the value.

Technical user manuals were not evaluated in detail to support the linkage analysis. Based on a review of the user manual, timescales are not stated but appear compatible. For example, flow from upstream to downstream segment is saved every day by default. Spatial resolution compatibility appears good. AQUATOX supports unidirectional and bi-directional flow of material from one segment to another. Networks can be built using a mixture of "cascading" and "feedback" links. Circular systems can also be simulated. All segments connected with feedback links are solved simultaneously, and cascading conglomerates of segments are solved sequentially going downstream. AQUATOX models up to 10 layers of bottom sediment.

### CE-QUAL-ICM

The water quality module (CE-QUAL-ICM) input and output is split across 16 input files and 11 output files. These files are organized along thematic lines. Code encapsulation could not be determined without a review of the source code, but the documentation in the user manual suggests the input and output routines are reasonably modular. Time scale and resolution is adjustable, as the model can write temporal averages to specified files at a specified time interval. Spatial resolution may pose a problem, as the model requires recompilation for any change in some of the structural parameters. Some of the parameters that require a recompilation of code are: number of grid cells, number of load sources, and maximum number of time varying input files. These parameters may need to be varied frequently in a coupling with a watershed model. Even if all coupling parameters were known in advance, a different executable will have to be maintained for each waterbody modeled.

### ECOM-3D/POM, ECOMSED

The model input and output is spread across 24 input files and 7 output files. All these files are well documented and organized along thematic lines into related parameter and time series data requirements. The organization of output data files is designed for integration with water quality models developed by the same firm. Filters for exchange with WWMS are possible but may not be necessary for internal interaction within components implemented as part of the ECOM suite. Code modularity appears good. Time and space scale and resolutions problems appear to have been addressed already. Level of detail of input and output can be adjusted. Scientific computations can be turned on and off. Overall, the model scores high on all criteria for compatibility with a WWMS.

### EFDC, EFDC1D

EFDC and EFDC1D may have the same requirements as CE-QUAL-ICM for recompilation for every new model geometry, because of its use of fixed dimension arrays. The most recent source code is available in the public domain but the user manual dates back to 1996, making it obsolete for current purposes as the model has undergone substantial enhancements since then in terms of its I/O capabilities. Other promotional materials are readily available and suggest that other than the recompilation requirement this model will have no problems of compatibility with WWMS.

### HSPF-RCHRES

HSPF uses WDM files as input and output, though other formats are also supported. Because the concept of a generalized dataset is intrinsic to this named model, its compatibility with a WWMS is expected to be the highest among other models reviewed. The time and space scales supported, as well as its scientific compatibility with WWMS is expected to be high because the model uses very detailed formulations. Compatibility with low complexity waterbody models will require use of carefully designed aggregation methods.

HSCTM-2D

The documentation of this model is excellent and compact, while including theory, operations, and an example problem. The ability to run the model with a “default option” adds to the compatibility score, though the caution necessary to use such an option may dictate that this option be disabled in a user level package. Input and output are split across several files as in most models. SMS can be used for pre-processing and post-processing some of these files. Number of files to be opened is itself an input parameter.

The input and output code appears to not be encapsulated very well. Some instances were encountered in the user manual where input from successive lines in the same input file occurred in different subroutines. This may not be a problem with use of wrappers when integrating this model within a WWMS.

IPX

IPX is a WASP derivative. Some of the hard-wired limits appear to have been removed or extended. The code and input/output data structures appear sufficiently modular. Pre-processors are also available. The model appears well documented at the level of detail necessary to attempt integration with WWMS.

Two additional segment types have been added over the WASP offerings. Bottom sediment surface layer and subsurface layers can now be added and subtracted in response to a sediment-water boundary that moves as a result of deposition or erosion. This is referred to as the semi-Lagrangian option. Transport processes appear to have been recoded and reorganized to remove the limit on number of solids that can be handled.

Scientific formulations remain similar to WASP. Overall, the compatibility of IPX with WWMS is expected to be higher than that of WASP.

WASP5

WASP5 has no watershed or hydrodynamic module. Flow fields can be supplied to WASP as a .HYD file from any proposed hydrodynamic module. Nonpoint source loading can be supplied similarly via a .NPS file. Sediment transport module of WASP is represented by its named module TOXI5. This module is driven by an ascii input file. It is not clear from the manual whether there are native file level data structures, or if input and output code are modular. Anecdotal evidence and a review of the input file format suggest that modifications and generalizations may be difficult to encode into the model, hence use of wrappers may be appropriate.

WASP has hard-coded numerical limits on the number of similar state variables, e.g., only three solid types are allowed. This may prove to be an impediment in generalizing the input and output of WASP into WWMS data structures. However, applications that otherwise could be run with WASP numerical limits may still be able to use WASP.

Time scales appear appropriate to coupling with a detailed watershed model like HSPF. There can be multiple segments and a complex network topology. Four types of segments are supported. Epilimnion, hypolimnion, upper benthic layer, lower benthic layer. Advection and dispersion are divided into six types: 1) advection and dispersion in the water column, 2) porewater flow through sediments and sediment-water exchange, 3) settling, resuspension, and sedimentation of three classes of solids, 6) evaporation or precipitation in each surface segment.

### 3.4.4 Evaluation Matrix

Table 3.12 shows the score of each candidate model in terms of its compatibility with WWMS when serving in its role as one of the four components. The score is on a three point scale of A, B, C. The score should be interpreted as follows:

A = excellent compatibility, no conceptual or operational problems expected.
B = mixed score, some effort may be required, but integration should be considered easy and doable.
C = integration appears difficult, and needs further careful study. It may eventually be found more efficient to recode the equations rather than try to reuse the existing model code
'-' = named model does not have this module

In some cases, a lowercase score is added to the '-' sign to indicate the "expected compatibility" of the named model, if the required module were to be added natively to the named model. This category was added because such an addition is frequently a relatively trivial exercise. It is assumed for purposes of this matrix that all the named models are being evaluated for modification at the source code level at EPA, and expertise for such modifications is readily available.

The rankings included in Table 3.12 are very preliminary assessments based in most cases on a quick review of the user manuals. The assessment may change as investigation proceeds and additional difficulties and corresponding work-arounds emerge during the integration.

Finally, the score indicates only the compatibility with the proposed watershed-waterbody modeling system. Other aspects of the model, e.g. ease of use, documentation, processes, are reviewed elsewhere.

Table 3.12. Preliminary Assessment of Compatibility of Selected Named Models

| | Hydrodynamic | Sediment F&T | Contaminant F&T | Conventional Pollutant F&T |
|---|---|---|---|---|
| AQUATOX | - | A | A | A |
| CE-QUAL-ICM | - | -,c | -,c | C |
| ECOM-3D/POM, ECOMSED | A | A | -,a | -,a |
| EFDC, EFDC 1-D | B | B | B | B |
| HSCTM-2D | B | B | B | - |
| HSPF-RCHRES | -,b | A | A | A |
| IPX | -,c | B | B | - |
| WASP5 | -,c | C | C | C |

# 4.0 CONCLUSIONS AND RECOMMENDATIONS

## 4.1 Model Science

Site-Specific ‘Conceptual Model’

Prior to initiating the development of any model for a site-specific contaminated sediment problem, it is essential that a ‘conceptual model’ be prepared to help guide the model selection process. The ‘conceptual model’, based on an inventory, compilation and analysis of the available site-specific data, identifies the most significant physical, biological and geochemical processes and interactions that control the transport and fate of solids and the toxicant(s) of concern. Of critical importance for the development of a site-specific model, the ‘conceptual model’ identifies the availability of data as well as any critical data gaps. In addition to the scientific data and information gathered, the ‘conceptual model’ clearly identifies the state, local or federal regulatory issues and/or resource management issues related to the contaminant of concern. The ‘conceptual model’ clarifies the purpose/objectives/goals of the intended contaminated sediment modeling study. Finally, the ‘conceptual model’ serves to identify the level of scientific detail required to support the decision-making process. The availability of site-specific data, the level of scientific detail required for technically credible decision-making, and the availability of skilled personnel and the resources allocated for the study, in turn, all enter into the selection of either intermediate level model(s) or advanced level model(s) for the contaminated sediment modeling framework.

Solids, Organic Carbon and Toxic Chemical Transport and Fate Models

The state of scientific knowledge incorporated in the advanced versions of hydrodynamic models, sediment transport models, toxic chemical transport and fate models and conventional pollutant models is at a very impressive level of detail. The representation of the details of specific processes, of course, will, and always can be improved. In all the models evaluated, however, one missing link stands out. Organic matter generated by biological models is not internally coupled with either sediment transport models or toxic chemical models. Distributions of dissolved (DOC) and particulate organic carbon (POC) that are needed for three-phase partition calculations in a toxic chemical model are empirically assigned as input data to parameterize the distributions of DOC and POC in the following toxics models: EFDC, EFDC1D, WASP-TOXI and IPX.

User-assigned settling velocities are used to parameterize the settling and deposition of algae and particulate organic carbon (POC) in biological models. A more rigorous approach would be to internally couple the sediment transport formulations used for deposition and resuspension of cohesive solids to describe settling, deposition and resuspension of biologically simulated algae and POC in the water column and bed.

With the exception of AQUATOX, dissolved (DOC) and particulate organic carbon (POC) in the water column and bed generated by a biological model is not internally coupled with the organic carbon-based three-phase partitioning model used in toxic chemical models. User-assigned distributions of POC or fractions of organic carbon (Foc) are combined with solids simulated by the sediment transport model to parameterize POC in the water column and bed. User-assigned distributions of DOC are input to describe DOC in the water column and bed.. A more rigorous approach would be to internally couple biologically simulated water column and bed DOC and

POC with the three-phase partition calculations in a toxics model.

Internal coupling of a biological model with sediment transport and toxic chemical models would, by eliminating the need for user-assigned parameterization of algae and POC settling rates, and distributions of POC and DOC, decrease the degrees of freedom presently allowed in the mass balance models for sediment transport, toxic chemicals and eutrophication.

The present approach for toxic chemical models, dependent on the modeler's parameterization of DOC/POC distributions and the fraction of organic carbon in the water column and bed, has been applied in numerous toxic chemical modeling studies over the past two decades. There are three key assumptions, implicit in the 'conceptual model' for these studies, that justifies the empirical parameterization of organic carbon data as input to a toxics model. The assumptions are: (1) seasonal/spatial patterns of biological production can be reliably described by repeatable patterns; (2) biologically produced organic matter is a minor component of the total solids budget; and (3) remediation alternatives are not expected to alter seasonal/spatial patterns of biological production.

If these key assumptions are not supported by the site-specific 'conceptual model' then a biological model should be internally coupled with the sediment transport and toxic chemical models to properly describe the interaction of DOC and POC with the three-phase partition calculations of the toxics model.

If there is a need to couple a biological model with a sediment transport model and a toxic chemical model to build a credible contaminated sediment model framework, the selection of an intermediate biological model (e.g., WASP-EUTRO) could provide an appropriate level of biological detail rather than a more complex advanced biological model (e.g., EFDC or CE-QUAL-ICM).

Of all the intermediate and advanced models evaluated for this study, implementation of these recommendations would be the most straightforward in EFDC. The EFDC model framework includes a toxics model and an advanced water quality/eutrophication model that is coupled with the hydrodynamics and sediment transport models. These recommendations could also be implemented in AQUATOX since the sediment transport sub-model of AQUATOX has been successfully tested and is considered to be operational by the model developers.

### 4.2 Model Support and Usability

(1) Lacking a universal description of what a User's Manual should contain, all the models were found to provide adequate documentation. Typical documents introduce the principles and concepts of each model, describe the foundations of the algorithms, and describe the input required to run the models. However, there is a clear need for improvements in documentation to include a step-by-step tutorial of model use in order for a user to exploit all of a model's capabilities.

(2) The models under consideration generally lacked in GUI's and GIS linkage, with the exception of WASP6 and HSPF-RCHRES. Most model developers recognize the advantages realized by implementing user interfaces, and propose to include GUI's and GIS linkage in upcoming versions. However, *ease* in applying complex models is a mixed blessing. While experienced model users are empowered to make faster and more powerful applications,

inexperienced users can fall into the trap of successfully running a model without fully understanding either (1) the background actions that the interface is performing in response to their instructions or (2) the underlying science that the model embodies.

(3) The degree and timeliness of human support available appears to vary widely. Realistically, the most comprehensive and consistent support appears to be available for a fee. Internet Listservers such as those provided for WASP and HSPF provide an effective means for modelers to help each other overcome obstacles encountered in their modeling efforts.

(4) Judging the application histories of the various models is complicated by the fact that most the models are evolving, and it is difficult to match application history to the specific scientific capabilities that were embodied in the version used for individual applications.

(5) The tools available for each model to perform data manipulation with the intent of providing the necessary input to each model (pre-processing) are not clearly documented or are outright lacking. While some models rely on third-party software (and its documentation) for pre-processing of data, description of the interface between the third-party tool and the model is generally not available.

(6) The tools available to perform post-processing of output data are also not clearly documented or outright lacking. Whether they are integrated with the GUI and GIS capabilities also seems to be unclear or missing completely in most model documentation.

### 4.3 Model Linkage

(1) A generic information exchange mechanism was proposed that would mediate the coupling between any two models within a watershed-waterbody modeling system (WWMS). This approach simplifies the investigation, and later implementation, of coupling between all possible pairs of models.

(2) Criteria for evaluating the linkage compatibility of models were identified. Two operational criteria (input/output encapsulation and code encapsulation) and three conceptual criteria (time resolution, space resolution, scientific compatibility) were identified as critical to linkage potential.

(3) The next step in further development of a watershed-waterbody linkage would be a detailed specification of the proposed generic information exchange structure. Such a specification will hypothesize a “dataset” as a fundamental unit of information. A comprehensive and hierarchical listing of required datasets, methods of query and storage of datasets, as well as methods of transformation of one dataset to another would form the high level specification. The low-level specification will be the implementation of these “dataset” structures and methods in a programming language. The evaluation criteria for each model would measure how comprehensively the model provides the components required in the WWMS and how much programming effort is required to provide these components. Compatibility of any candidate pair of models could be assessed by how well the inputs of one match the datasets made available by the outputs of the other.

WWMS is proposed as an inclusive, not an exclusive approach. An integration approach that excludes some models and includes only a few of available useful models implies the use of a ranking method. No ranking method can be so universal so as to apply to all combinations of problem definitions and available resources encountered in environmental studies being done in the world. A named waterbody model likely exists because it was previously found useful in some applications. Thus a WWMS should facilitate, and not prevent, integration of all existing waterbody models with the watershed model most compatible to their specific input needs.

(4) If a model does not score very high on operational compatibility, it can be included in the system by use of wrappers/filters. Such middleware can be constructed by the developer or experienced users, effectively distributing the programming and maintenance effort without losing conformity to each other. For modular and generalized models like HSPF, it may be more appropriate to skip the middleware step, and recode them to exchange information natively to/from the WWMS.

(5) If a model does not score very high on conceptual compatibility with a large number of other models, its presence in the WWMS suite would not impose any programming or run-time overhead on models that do not use inputs from it. In this sense, the WWMS is intended as an all-inclusive approach. Models that don’t fit very well with other models because of non-standard process formulations or non-standard file input and output, nevertheless may be the most appropriate models for some problem definitions.

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# APPENDIX A: MODEL SCREENING RESULTS

Tables A.1 through A.4 present the results of the preliminary screening of the candidate models. A unique set of screening criteria were applied to each of the four modeling component groups that determine contaminated sediment transport and fate. Note that the Study Team eliminated additional modeling components using subsequent information gained by discussions with the model developers. The models selected for detailed evaluation by this final screening are reported in Section 3.1.2.

| | General | | | | Hydrodynamics | | | |
|---|---|---|---|---|---|---|---|---|
| | Availability | Human Model Support | Documentation | Application History | Linkage to Sediment Transport & Toxic Fate Models | Model Formulation | Initial Conditions | Boundary Conditions and External Forcing Functions |
| | G1 | G2 | G3 | G4 | H1 | H2 | H3 | H4 |
| ADCIRC | X | | | | X | | | |
| AQUASEA | X | | | | | | | |
| BFHYDRO | x | | | | | | | |
| Branch | | | | | X | | | |
| C3 | X | | | | | | | |
| **CE-QUAL-RIV1** | | | | | | | | |
| **CE-QUAL-W2** | | | | | | | | |
| **CH3D/WES** | | | | | | | | |
| CORMIX | | | | | X | X | | |
| DYNHYD5 | | | | | X | X | | |
| **ECOM-3D** | | | | | | | | |
| **EFDC** | | | | | | | | |
| **EFDC-1D** | | | | | | | | |
| FESWMS-2D | | | | | x | | | |
| FLDWAV2.0 | | | | | x | | | |
| FLOW-DELFT3D | x | | | | | | | |
| GEMSS-HDM | X | | | | | | | |
| HEC-2 | | | | | | X | | |
| HEC-RAS | | | | | | X | | |
| **HSCTM-2D** | | | | | | | | |
| MECCA | | | | | X | | | |
| MIKE11 | X | | | | | | | |
| MIKE21 | X | | | | | | | |
| MIKE3 | X | | | | | | | |
| MODFLOW-HMS | X | | | | | | | |
| Peter Sheng | X | | | | | | | |
| **POM** | | | | | | | | |
| **RIVMOD** | | | | | | | | |
| RMA-10 | X | | | | | X | | |
| RMA-2 | X | | | | | X | | |
| Sobek | X | | | | | | | |
| TABS-2 | | | | | | X | | |
| TELEMAC-3D | X | | | | | X | | |
| TIDE3D/XTIDE3D | | X | | X | | | | |
| TRIM3D | X | | | | | | | |
| TRIVAST | X | | | X | | | | |
| UNET | X | | | | | | | |
| Wenrui Huang | X | | | | X | | | |

**Table A.1** Hydrodynamic Models. Models passing screening are indicated in bold. However, CE-QUAL-RIV1 and RIVMOD are also eliminated because their modeling components other than hydrodynamics did not pass screening.

| | Availability | Human Model Support | Documentation | Application History | Conservation of Mass | Coupling of Water Column & Sediment Bed | Spatial Dependence of Initial Conditions | Point & Nonpoint Source Boundary Inputs | Linkage to Toxic Chemical Fate Model |
|---|---|---|---|---|---|---|---|---|---|
| | General | | | | Sediment Transport | | | | |
| | G1 | G2 | G3 | G4 | S1 | S2 | S3 | S4 | S5 |
| AQUASEA | x | | | | | | | | |
| **AQUATOX** | | | | | | | | | |
| BFWASP | x | | | | | | | | |
| C3 | x | | | | | | | | |
| **CE-QUAL-ICM/TOXI** | | | | | | | | | |
| CE-QUAL-W2 | | | | | x | x | | | |
| CH3D-SED | x | | | | | | | | |
| CORMIX1,2 | | | | | x | x | | | |
| CTAP | | | | | x | | | | |
| DELFT3D | x | | | | | | | | |
| **ECOMSED** | | | | | | | | | |
| **EFDC** | | | | | | | | | |
| **EFDC-1D** | | | | | | | | | |
| GEMSS-STM | x | | | | | | | | |
| GSTARS | | | | | | | | | x |
| HEC-6 | | | | | x | | x | | x |
| **HSCTM-2D** | | | | | | | | | |
| **HSPF-RCHRES** | | | | | | | | | |
| HUDTOX | | | | x | | | | | |
| **IPX Vers 2.7.4** | | | | | | | | | |
| ISIS | x | | | | | | | | |
| MICHRIV | | | | | x | | | | |
| MIKE11/21 | x | | | | | | | | |
| MIKE3-WQ | x | | | | | | | | |
| RIVMOD | | | | | x | x | | | x |
| RMA11 | x | | | | x | | x | | |
| **SEDZL** | | | | | | | | | |
| SERATRAWASP5 | | | | x | | | | | |
| SLSA | | | | | x | | | | |
| SMPTOX3 | | | | | x | | | | |
| Sobek | x | | | | | | | | |
| SSFATE | x | | | | | | | x | |
| SED2D-WES | x | | | | | | | | |
| TRIM2D/TRIM3D | x | | x | | | | | | |
| TSEDH/RMA2 | | | x | | x | | | | |
| WAQ-DELFT3D | x | | | | | | | | |
| **WASP5(6)-TOXI5(6)** | | | | | | | | | |

**Table A.2** Sediment Transport Models. Models passing screening are indicated in bold.

| | General | | | | Toxic Chemical Transport and Fate | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Availability | Human Model Support | Documentation | Application History | Conservation of Mass | Coupling of Water Column & Sediment Bed | Kinetic Processes and Interactions | Spatial Dependence of Initial Conditions | Point and Nonpoint Source Boundary Inputs | Linkage with Sediment Transport Model |
| | G1 | G2 | G3 | G4 | T1 | T2 | T3 | T4 | T5 | T6 |
| **AQUATOX** | | | | | | | | | | |
| BFHYDRO/WQMAP | X | | | | | | | | | |
| C3 | X | | | | | | | | | |
| **CE-QUAL-ICM-TOXI** | | | | | | | | | | |
| CE-QUAL-W2 | | | | | X | X | X | X | X | X |
| CHEMMAP | X | | | | | | | | | |
| CTAP | | | | | X | | X | | | |
| DELFT3D-WAQ | X | | | | | | | | | |
| **EFDC** | | | | | | | | | | |
| **EFDC-1D** | | | | | | | | | | |
| EXAMS | | | | | X | | | | | |
| GBTOX/GBOCS | | | | X | | | | | | |
| GEMSS-WQM | X | | | | | | | | | |
| **HSCTM-2D** | | | | | | | | | | |
| **HSPF-RCHRES** | | | | | | | | | | |
| HUDTOX | | | | X | | | | | | |
| **IPX Vers 2.7.4** | | | | | | | | | | |
| MICHRIV | | | | | X | | X | | | |
| MIKE-11 | X | | | | | | | | | |
| MIKE12 | X | | | | | | | | | |
| MIKE-21 | X | | | | | | | | | |
| MIKE3-WQ | X | | | | | | | | | |
| Peter Sheng | X | | | | | | | | | |
| QWASI | | | | | | | X | | | |
| RATECON | | | | X | | | | | | |
| **RCA-TOX** | | | | | | | | | | |
| RIVRISK | | | | | | | X | | | |
| RMA11 | X | | | | X | | | | | |
| SAGEM | | | | X | | | | | | |
| SLSA | | | | | X | | X | | | |
| SMPTOX3 | | | | | X | | X | | | |
| SMPTOX4 | | | | | X | | X | | | |
| TELEMAC-3D | X | | | | X | | | | | |
| TIDE3D/XTIDE3D | | X | | X | | X | | | | |
| TOXIROUTE | | | | | X | | X | | | |
| TRIVAST | X | | | X | | | | | | |
| **WASP5(6)-TOXI5(6)** | | | | | | | | | | |
| **WASTOX** | | | | | | | | | | |
| Wenrui Huang | X | | | | | | | | | X |
| WQAM | | | | | X | | X | | | |

**Table A.3** Toxic Chemical Transport and Fate Models. Models passing screening are indicated in bold.

| | Availability | Human Model Support | Documentation | Application History | Conservation of Mass | Coupling of Water Column and Sediment Bed | Kinetic Processes and Interactions | Spatial Dependence of Initial Conditions | Point and Nonpoint Source Boundary Inputs | Linkage of SS to Eutrophication Models | Linkage of SS & OC to Contaminant Fate Models |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | **General** | | | | Conventional Pollutants and Eutrophication | | | | | | |
| | **G1** | **G2** | **G3** | **G4** | **C1** | **C2** | **C3** | **C4** | **C5** | **C6** | **C7** |
| ADYN/RQUAL | | | | | | | x | | | | |
| **AESOP** | | | | | | | | | | | x |
| AQUAMOD | | | | | | | x | | | | |
| **AQUATOX** | | | | | | | | | | | x |
| BATHTUB | | | | | x | | | | | | |
| BETTER | | | x | x | | | | | | | |
| BFWASP/WQMAP | x | | | | | | | | | | |
| C3 | x | | | | | | | | | | |
| **CE-QUAL-ICM** | | | | | | | | | | | x |
| CE-QUAL-R1 | | | | | | | | | | x | x |
| CE-QUAL-RIV1 | | | | | | | | | | x | x |
| **CE-QUAL-W2** | | | | | | | | | | | x |
| CORMIX | | | | | | x | x | | | | |
| DECAL | | | | | | | x | | | | |
| DSSAMt | x | | | | | | | | | | |
| ECOFATE | | | | | | | x | | | | |
| **EFDC** | | | | | | | | | | | x |
| **EFDC-1D** | | | | | | | | | | | x |
| EHSM3D | | | | | | | x | | | | |
| EUTROMOD | | | | | x | | | | | | |
| GEMSS-WQM | x | | | | | | | | | | x |
| HEC5Q | | | | | | | x | | | | |
| HOTDIM | | | | | | | x | | | | |
| **HSPF-RCHRES** | | | | | | | | | | | x |
| HYDRO 2D-V | | | | | | | x | | | | |
| HYDRO 3D | | | | | | | x | | | | |
| ISIS | x | | | | | | | | | | |
| John Paul's model | | | | | | | x | | | | |
| LIMNOD | | | | | | | x | | | | |

**Table A.4** Conventional Pollutant Transport and Fate and Eutrophication Models. Models passing screening are indicated in bold. Note that the C7 criterion was eliminated after being judged too restrictive.

| | Availability | Human Model Support | Documentation | Application History | Conservation of Mass | Coupling of Water Column and Sediment Bed | Kinetic Processes and Interactions | Spatial Dependence of Initial Conditions | Point and Nonpoint Source Boundary Inputs | Linkage of SS to Eutrophication Models | Linkage of SS & OC to Contaminant Fate Models |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | General | | | | Conventional Pollutants and Eutrophication | | | | | | |
| | G1 | G2 | G3 | G4 | C1 | C2 | C3 | C4 | C5 | C6 | C7 |
| MBM | | | | | | | x | | | | |
| MECCA | | | | | | | x | | | | |
| MIKE11 WQ | x | | | | | | | | | | |
| MIKE21 WQ | x | | | | | | | | | | |
| MIKE3-WQ | x | | | | | | | | | | |
| MODFLOW-HMS | x | | | | | | | | | | |
| PCPROUTE | | | | | | x | x | | | | |
| Peter Sheng's model | | | | | | | x | | | | |
| PHOSMOD | | | | | x | | | | | | |
| PLUMES | | | | | | x | x | | | | |
| QUAL2E | | | | | | x | | | | x | x |
| **RCA** | | | | | | | | | | | |
| REACHSCAN | | | | | | | x | | | | |
| RMA11 | x | | | | | | | | | | |
| SALMONQ | x | x | | | | | | | | | |
| SEDDEP | | | | | | | x | | | | |
| SIM-PEL | | | | | | | x | | | | |
| Sobek | x | | | | | | | | | | |
| TELEMAC-3D | x | | | | | | | | | | |
| TEMPEST | | | | | | | x | | | | |
| TPM | | | | | | | x | | | | |
| TPWQM | | x | | | | | | | | | |
| TRIVAST | | | | | | | x | | | | |
| TWQM | | | | | x | | | | | | |
| WAQ-DELFT3D | x | | | | | | | | | | |
| WARMF | x | | | | | | | | | | |
| **WASP5(6)-EUTRO5(6)** | | | | | | | | | | | x |
| Wenrui Huang's model | | | | | | | x | | | | |
| WQAM | | | | | | | x | | | | |
| WQMAP | x | | | | | | | | | | |
| WQRRS | | x | | x | | | | | | | |
| XTIDE3D | | | | | | | x | | | | |

**Table A.4 (concluded)** Conventional Pollutant Transport and Fate and Eutrophication Models. Models passing screening are indicated in bold. Note that the C7 was eliminated after being judged too restrictive.

## APPENDIX B: WATERBODY DESCRIPTIONS

Physical descriptions for nine waterbody types are provided in this appendix. Included are:

(1) Free-flowing freshwater streams
(2) Freshwater rivers
(3) Tidal rivers
(4) Well-mixed lakes
(5) Stratified lakes and reservoirs
(6) Well-mixed tidal embayments
(7) Stratified narrow estuaries
(8) Stratified broad estuaries
(9) Coastal ocean

*Free-flowing Freshwater Streams: 1D(x).* Streams are classified as low-order channels with a steep bottom gradient that results in a relatively high-velocity, shallow stream characterized by gravel, cobbles and rocks in the stream bed. Coarse sands and finer particles are washed out by the high velocity conditions. Multiple branched low order streams interact by hydrologic routing. The dominant gradient of water quality constituents is along the longitudinal axis in the direction of flow. A one-dimensional laterally and vertically averaged model is thus appropriate for describing flow of water and the mass transport of solids and toxic chemicals. Transport in many streams is characterized as an inertia dominated waterway since the mean velocity of the stream exceeds the speed (celerity) of a gravity wave. Transport in such a free-flowing stream can be appropriately represented using a kinematic wave hydraulic model. The key feature of a kinematic wave model is that the slope of the free water surface matches the slope of the stream bed. The practical implication of this hydraulic condition is that downstream conditions do not exert an influence upstream on velocity or depth. In a free-flowing stream, backwater effects are not present. Based on the Peclet number, mass transport in a stream is dominated by advection with dispersion determined to account for a minor component of the mass flux of a constituent. Dispersion can thus be neglected in a stream model. Time variable upstream boundary conditions of flow and/or stage elevation must be able to be assigned for a kinematic hydraulic model of a stream.

*Freshwater Rivers: 1D(x).* Rivers are classified as higher order channels located in alluvial and lowland valleys with a moderate bottom gradient. The low grade of the river bed results in a low-velocity waterway characterized by a sediment bed consisting of a mixture of fine grained cohesive particles and fine sands. The dominant gradient of water quality constituents in many rivers is along the longitudinal axis of flow. A one-dimensional laterally and vertically averaged model can thus be appropriate for describing the flow of water and the mass transport of solids and toxic chemicals in many rivers of moderate width and depth. Transport in rivers is characterized by sub-critical flow with a Froude number <1. Transport in a river, dominated by the influence of downstream backwater effects, can be appropriately represented using a dynamic hydraulic model. The key feature of a dynamic model of sub-critical flow is that the free water surface is allowed to pile up and increase the depth of the water column in the upstream direction. The practical implication of this hydraulic condition is that downstream conditions can exert a considerable influence on upstream velocity and depth through the backwater effects of a dam, impoundment or some other blockage (e.g., debris) to flow in a moderate gradient river. Based on the Peclet number, mass transport in a river, especially the larger, high order rivers, is characterized by advection and dispersion, both accounting for comparable magnitudes of the mass flux of a constituent. Dispersion must therefore be represented in a model applied to rivers. Time variable upstream and downstream boundary conditions of flow and/or stage elevation must be able to be assigned for a dynamic hydraulic model of sub-critical flow in a river. In wide, deep higher order rivers, such as the Ohio River, the Missouri River and the Mississippi River, transport can be characterized by significant water quality gradients either laterally or vertically. The presence of significant lateral or vertical gradients for a water quality constituent such as chlorides or suspended solids, for example, would require the application of a two- or a three-dimensional hydrodynamic model rather than a one-dimensional hydraulic model.

*Tidal Rivers: 1D(x).* Tidal rivers are defined as relatively narrow and shallow waterways with transport controlled by freshwater inflow at the upstream boundary and tidal forcing of water surface elevation at the downstream boundary. Tidal rivers, particularly small rivers and creeks that flow into an estuary or bay (e.g., Christina River flowing into Delaware estuary), can often be appropriately characterized as a one-dimensional river where lateral and vertical water quality gradients are negligible. Since the downstream boundary condition of tidal fluctuation in water surface elevation influences upstream velocity and stage height, the class of one-dimensional hydraulic models presented above for high-order freshwater rivers are also applicable to tidal rivers. Based on the Peclet number, mass transport in a tidal river can be characterized by both advection and dispersion accounting for comparable magnitudes of the mass flux of a constituent or dispersion can account for the dominant mass flux component. In a tidal river, advection and dispersion must both be represented. Time variable upstream boundary conditions of flow and/or stage elevation and downstream boundary conditions of the tidal forcing of water surface elevation must be able to be assigned for a one-dimensional model of flow in a tidal river. In large tidal rivers, such as the Lower Hudson River and the Lower Potomac estuary, transport can be characterized by significant water quality gradients either laterally, vertically or both. The presence of significant lateral or vertical gradients of salinity in a tidal river from freshwater inflows, wind forcing or bottom water salt intrusion requires application of a two- or a three-dimensional hydrodynamic model rather than a one-dimensional hydraulic model. The application of an one-dimensional model to a tidal river characterized by pronounced lateral or vertical gradients of salinity (i.e., either partially of fully stratified) is not an appropriate choice.

*Well-Mixed Freshwater Lakes and Bays: 2D(xy).* A well-mixed freshwater lake, or an embayment of a large lake, is typically classified as a relatively broad and shallow body of water. Horizontal water quality gradients in broad, shallow lakes, arising from winds and inflows of freshwater, are almost always significant along the lateral and longitudinal directions of transport. Because of vigorous vertical mixing in shallow water, vertical gradients of water quality constituents are minimal. For “broad” and “shallow” lakes, two-dimensional, vertically averaged [2D(xy)] models of circulation are appropriate where circulation is governed by winds, freshwater inflow, the geometry of the shoreline, basin bathymetry and the flow control structure at the outlet end of the lake. For a well-mixed lake, the low value of the Richardson number is indicative of a stable water column with a negligible vertical temperature gradient. Where field data and the ‘conceptual model’ demonstrate a stratified water column, then a two-dimensional, depth-averaged model is not an appropriate choice; a three-dimensional model is required to represent such conditions. An one-dimensional hydraulic model is most certainly not an appropriate choice for a well-mixed lake characterized by horizontal gradients of water quality. In a two-dimensional, depth averaged hydrodynamic model of a shallow lake, advection and dispersion must both be represented in the horizontal dimensions. Horizontal dispersion coefficients, at a minimum, must be defined by appropriate length scale empirical formulations. Time variable upstream and lateral boundary conditions of flow and/or stage elevation and downstream boundary conditions for the outlet of either flow and/or a rating curve of stage height and flow must be able to be assigned for a two-dimensional, depth-averaged model of flow in a shallow lake.

*Stratified Lakes and Reservoirs: 2D(xz).* Freshwater lakes and reservoirs are classified as relatively flat bodies of water characterized by relatively large surface areas. With one or more upstream inflows and a downstream outlet, water quality gradients in lakes and reservoirs are almost always significant along the longitudinal axis of transport. Because of deep water conditions and restricted vertical mixing in many lakes and reservoirs, vertical gradients of water quality constituents can arise from seasonal winter-summer stratification and/or from inflows of cold water rivers into a warmer water lake or reservoir. For "narrow" and "deep" lakes (e.g., Finger Lakes in New York State) and reservoirs, two-dimensional, laterally averaged [2D(xz)] models of circulation can be appropriate where transport is governed by winds, vertical density gradients, freshwater inflow, the geometry of the shoreline, basin bathymetry and the flow control structure(s) at the outlet end of a lake or reservoir. For a stratified lake or reservoir, the high value of the Richardson number would be indicative of an unstable water column with significant vertical temperature gradients. An one-dimensional hydraulic model is not appropriate for a lake or reservoir. For some lakes and reservoirs characterized by a large surface area, lateral gradients in water quality may be a significant feature that requires selection of a three-dimensional hydrodynamic model. In a two-dimensional, laterally averaged hydrodynamic model of a lake or reservoir, advection and dispersion must both be represented in the longitudinal and vertical dimensions. Horizontal and vertical dispersion coefficients, at a minimum, must be defined by appropriate length scale empirical formulations. One-equation and two-equation methods can provide increasingly realistic approximations for horizontal and vertical diffusivity estimates required by turbulence closure. Time variable upstream and lateral boundary conditions of flow and/or stage elevation and downstream boundary conditions for a control structure based on a rating curve of stage height and flow over the outlet must be able to be assigned for a two-dimensional laterally averaged model of flow in a lake or reservoir.

*Well-Mixed Tidal Bays: 2D(xy).* A well-mixed tidal embayment is typically classified as a relatively broad and shallow body of water influenced by tidal forcing at the open boundary of the bay. Horizontal water quality gradients in shallow bays, such as the bays and lagoons inshore of the barrier islands on the east coast from Long Island to Cape Hatteras, arise from winds, tidal exchange and, possibly inflows of freshwater, are almost always significant. Because of vigorous vertical mixing in shallow bays, primarily from tidal mixing, vertical gradients of salinity and other water quality constituents are minimal. For "broad" and "shallow" bays, a two-dimensional, vertically averaged [2D(xy)] model of circulation is an appropriate choice where circulation is governed by winds, freshwater inflow, the geometry of the shoreline, basin bathymetry and the tidal forcing across the open boundary of the bay. For a well-mixed bay, the low value of the Richardson number is indicative of a stable water column with small salinity and temperature gradients. In a two-dimensional, depth averaged hydrodynamic model of a shallow bay, advection and dispersion must both be represented in the horizontal dimensions. Horizontal dispersion coefficients, at a minimum, must be defined by appropriate length scale empirical formulations that reflect tidal mixing processes. Time variable upstream and lateral boundary conditions of flow and/or stage elevation and the open boundary condition allowing for the tidal variation of sea surface elevation must be able to be assigned for a two-dimensional, depth-averaged model of flow in a shallow coastal bay. Where field data and the ‘conceptual model’ demonstrate a stratified water column in a coastal bay, then a depth-averaged model is not an appropriate choice; a three-dimensional model is required to represent such conditions. A one-dimensional hydraulic model is most certainly not an appropriate choice for a well-mixed bay defined by horizontal gradients of water quality.

*Stratified “Narrow” Estuaries: 2D(xz).* Many “narrow” estuaries, including very deep fjords, are characterized by strong or partially stratified conditions arising from freshwater inflow at the upstream boundary flowing seaward in the surface layer and tidal forcing of heavier salt water flowing landward along the bottom layer from the downstream open boundary with the ocean. In a stratified estuary, such as the Patuxent River, a two-dimensional, laterally averaged [2D(xz)] model of circulation can be appropriate where transport is governed by winds, vertical density gradients, freshwater inflow, the geometry of the shoreline, basin bathymetry and tidal forcing at the open boundary with the ocean or larger estuary such as Chesapeake Bay. In a two-dimensional, laterally averaged hydrodynamic model of a stratified estuary, advection and dispersion must both be represented in the longitudinal and vertical dimensions. Horizontal and vertical dispersion coefficients, at a minimum, must be defined by appropriate length scale empirical formulations. One-equation and two-equation methods provide increasingly realistic approximations for horizontal and vertical diffusivity estimates required by turbulence closure. Time variable upstream and lateral boundary conditions of flow and/or stage elevation and tidal forcing of sea surface elevation at the downstream open boundary must be able to be assigned for a two-dimensional, laterally averaged model of flow in a stratified estuary.

*Stratified “Broad” Estuaries: 3D(xyz).* “Broad” estuaries and other tidal bodies of water characterized by sharp horizontal and vertical gradients of salinity should be represented with a three-dimensional hydrodynamic model. Advection and dispersion must both be represented in the horizontal and vertical dimensions. Horizontal and vertical dispersion coefficients, at a minimum, must be defined by appropriate length scale zero-order empirical formulations. One-equation and two-equation methods provide increasingly realistic approximations for horizontal and vertical diffusivity estimates required by turbulence closure in three-dimensional models. Time variable upstream and lateral boundary conditions of freshwater inflow and/or stage elevation and tidal forcing of sea surface elevation and salinity at the downstream open boundary of the estuary must be able to be assigned for a three-dimensional model of flow in a stratified estuary. Hydrodynamic models appropriate for simulation of estuarine circulation are essentially identical to models that would be chosen for coastal and open ocean hydrodynamic models. The key difference between an ocean and estuary model is that, because of the smaller spatial scale of an estuary (compared to the ocean), it is not necessary to select a hydrodynamic model that accounts for the rotation of the earth using the artificial Coriolis ‘force’.

*Coastal Ocean: 3D(xyz).* The key characteristics of the coastal ocean that must be represented in a hydrodynamic model include sharp horizontal and vertical gradients of salinity and other water quality constituents and the need to represent a coastline defined by an open offshore boundary at the continental shelf break and ‘upstream’ and ‘downstream’ open boundaries. Sharp density gradients result from the inflow of freshwater rivers into the coastal ocean and the mixing of the freshwater with salt water of the open ocean. Horizontal salinity and density gradients tend to parallel the bottom contours of the continental shelf. Pronounced cross-shelf vertical gradients of salinity, temperature and nutrients also arise from wind forcing and resulting onshore and offshore flow from coastal upwelling and downwelling (see Walsh, 1988). Advection and dispersion must both be represented in the horizontal and vertical dimensions. Horizontal and vertical dispersion coefficients, at a minimum, must be defined by appropriate length scale zero-order empirical formulations. One-equation and two-equation methods provide increasingly realistic approximations for horizontal and vertical diffusivity estimates required by turbulence closure in a three-dimensional model. Although tidal forcing at the open boundaries can be represented in coastal ocean models, the more important boundary condition is the specification of the spatial gradient of longshore and cross-shelf sea surface elevations at the offshore, upstream and downstream open boundaries. In the Middle Atlantic Bight, for example, there is a difference of approximately 10 to15 cm in sea surface elevation over ~700 km from Cape Cod to Cape Hatteras that drives the mean southwest current of ~3 to 5 cm/sec. In addition to the description of sea surface elevation as an open boundary condition, time variable boundary inputs of river discharge from the coast must be able to be assigned for a three-dimensional model of circulation in the coastal ocean. A full three-dimensional model of coastal ocean circulation should account for both the barotropic and baroclinic components of flow. The Rossby number, a ratio of the inertial and Coriolis acceleration terms in the equations of motion, indicates that the Coriolis term must be incorporated in the hydrodynamic model to account for rotation of the earth when the Rossby number is <<1 (see Walsh, 1988).

# APPENDIX C: WORK ASSIGNMENT QA/QC

This section describes the QA/QC goals for this study and the procedures that were used to achieve these goals.

The QA/QC goals for a model evaluation study such as this are as follows:

- Objectivity: To the fullest extent possible, all elements of the study should be performed objectively. In particular, the screening of models must be based on clearly stated, objective criteria. Selection of a model component as 'superior' and suited for use in ERD's planned R&D activities should not be based on criteria that cannot be explicitly stated and applied.
- Thoroughness: All elements of the study should be carried out and documented in a thorough manner. The effort made to identify a comprehensive list of models for screening should investigate a broad range of sources and references. The evaluation of models should include personal contact with model developers to verify and expand the Study Team's conclusions.
- Consistency: Work performed in each element of the study should be performed in a consistent manner. It should be a goal of the Study Team to treat all models in an equal fashion, and to avoid inadvertently 'skewing' the results, and the documentation of the results, because of greater personal familiarity with particular models.

Achieving the goals of objectivity, thoroughness and consistency in the efforts performed for this study was assured by the active participation of investigators from three different, loosely-associated firms. This approach to performing the work encouraged active debate and cross-checking of assumptions and results.

Successful completion of this study required the following activities:

- Developing screening criteria
- Developing comparison criteria
- Identifying models to be screened
- Applying screening criteria to identify superior models
- Performing detailed model evaluation
- Developing recommendations
- Evaluating model linkage approaches
- Documenting results

In the following sections we describe the procedures to which we adhered in order to assure our QA/QC goals were achieved while performing each of the required activities.

C.1 Developing Screening Criteria

Several recent studies (HydroGeoLogic, 1999; Tetra Tech, 2000) have effectively applied a multi-tiered evaluation approach in order to identify and compare models. The first-tier analysis applies a set of minimum requirements to all candidate models that considers the science of the models, the intended use of models and the models' usability. By tightening or loosening the minimum requirements, it is possible to generate a list of qualified models that is not so large in size that it hinders the subsequent process of performing a meaningful head-to-head comparison between the most promising models. The QA/QC component for developing screening criteria was comprised of the following:

- Each of the three participating firms reviewed and considered recent key documents that provided a sound basis for differentiating between contaminated sediment modeling components. Investigators considered the appropriateness of suggested screening criteria in the context of the current study.
- Each of the three participating firms developed a separate list of recommended screening criteria. The lists were compiled, and discussed by the Study Team to reach consensus on the best possible list for performing the initial screening.
- To the fullest extent possible, the screening criteria were explicit in nature, thus allowing the screening of models in a straightforward manner, with very limited interpretation on the part of the model reviewers.
- The screening criteria were clearly presented in a report suitable for consideration by the EPA WAM.
- The screening criteria were reviewed by the EPA WAM to make sure that they were consistent with EPA's goals in performing the model evaluation.
- The Study Team further scrutinized the remaining models, primarily by means of personal contact with the model developers. These correspondences uncovered a number of issues that had not been fully considered during the initial screening. Armed with the additional information gained by discussions with the model developers, the Study Team and the WAM eliminated additional modeling components to establish the final list of models for detailed comparison.

C.2 Developing Comparison Criteria

As was the case with the first-tier screening criteria, second-tier comparison criteria include scientific considerations, and also model support and usability issues. The scientific criteria are, of course, specific to each model class, whereas the model support and usability criteria are relevant to all models in all classes. Generally speaking, the second-tier assessment of the science of candidate models focused on (a) the capability of a candidate model to represent a key feature, attribute, process or interaction; and (b) the level of detail of the formulation(s) used to describe the processes or interactions. In numerous cases, the scientific comparison criteria identified in this section were lumped in nature. Many of these criteria were transformed into more specific criteria, sometimes at a state variable or process level of detail, after the qualifying models had been selected via the first-tier screening process.

The QA/QC component for developing comparison criteria was comprised of the following:

- Each of the three participating firms reviewed and considered recent key documents that provide a sound basis for characterizing, and differentiating between, contaminated sediment modeling components.
- Each of the three participating firms developed a separate list of recommended comparison criteria. The lists were compiled, and discussed by the Study Team to reach consensus on the best possible composite list for performing the initial comparisons.
- An initial list of criteria, some of which were lumped in nature, were provided to the EPA WAM in a report, and the criteria were modified and enhanced in response to the WAM's

comments.

- As the detailed comparison of selected models was carried out, the Study Team broke down lumped criteria into more specific state variable and process oriented comparison criteria. In addition, individual investigators identified and suggested additional useful enhancements to the comparison criteria. The Study Team decided on changes to the comparison criteria jointly.
- As many comparison criteria as possible were characterized using Yes/No connotations. Model component comparisons were captured in a series of matrices that explicitly compared models on a state-variable-by-state variable and process-by-process level.
- Certain of the comparison criteria that did not lend themselves well to the ‘yes-no’ characterization were characterized using small amounts of clearly worded text. For example, information characterizing the extent of model usage or model support could not be adequately conveyed in a ‘yes-no’ format.
- The final comparison criteria by which the selected models were compared were reviewed by all Study Team investigators one last time to be sure that they were appropriate and comprehensive prior to submitting a draft final report of the study's results to the EPA WAM.

C.3 Identifying Models to be Screened

This element of the study entailed the identification of a comprehensive list of currently existing contaminated sediment modeling components. The study approach was to identify as many models as possible that included one or more of the following components: sediment transport, toxic chemical transport and fate, conventional pollutant transport and fate. Within the context of this study our interest in hydrodynamic models is restricted to identifying the best models that are commonly used to drive the transport computations contained in the "best" sediment and chemical models. Consequently, the hydrodynamic models were selected subsequent to the identification of the sediment and chemical models.

The approach to identifying models was to first focus attention on recent reviews and compendia of models. By doing so, immediate recognition was gained of the most credible and commonly used models. The study work plan identified four very good references (Tetra Tech, 2000; HydroGeoLogic, 1999; Fitzpatrick, 2001; WEST Consultants, 1996) to support this effort. These resources, all of which represent recent (1995 or later) efforts to identify the best of the currently available modeling tools, and all of which were prepared by professionals actively involved in water quality modeling, provided a strong starting point for identifying candidate models. To ensure that the search for the most promising models was comprehensive, additional models were investigated by means of phone calls to knowledgeable professionals, and by investigating a set of well-organized and comprehensive internet links provided on the USGS Surface-water quality and flow Modeling Interest Group (SMIG) web page. In addition, each of the participating firms used additional reference materials within their firms' libraries to supplement the search.

The QA/QC component for identifying the models that were screened was comprised of the following:

- Each of the three participating firms developed a separate list of models, organized by modeling component, for screening.
- The search effort, and the sources identified and reviewed, was documented.
- The lists were then compiled to produce a comprehensive list for each modeling

component.

## C.4 Applying Screening Criteria to Identify Selected Models

Perhaps the most important QA/QC issue of the entire study pertains to assuring that a consistent and objective procedure was used for selecting the modeling components that were judged the most useful for ERD's purposes and carried forward in the study for detailed comparison. As stated before, the success of achieving this goal was largely determined by the careful selection and definition of the screening criteria. To the extent that the model evaluators could apply the screening criteria to candidate models without ambiguity, the screening results were considered correct and defensible.

In performing the initial screening, a "one strike and you're out" approach was used. During the screening process, as soon as a model failed one criterion, documentation of this failure was made, and the model was not further considered. This approach is consistent with the primary objective of the study, which is to identify and thoroughly compare a small number of the most suitable models for ERD to consider in carrying out its research goals.

The QA/QC component for applying the screening criteria to identify the 'best' models was comprised of the following:

- Each of the three participating firms applied the screening criteria to each of the following modeling components: sediment transport, toxic chemical transport and fate, and conventional pollutant transport and fate. A customized set of criteria were used for each component.
- The lists of surviving models identified by investigators were compiled and compared. Inconsistencies were resolved. At least one failed criterion for each model component excluded from the detailed analysis was documented.
- Each of the three participating firms applied the screening criteria for hydrodynamics models; and added a criterion that each candidate model must have a historical linkage to one or more of the selected sediment or chemical models.
- The Study Team checked the number and variety of models that satisfied <u>all</u> screening criteria in each component group. If both intermediate and complex models had survived the screening, and the total number of surviving models for each component group was between five and twelve, the screening process was considered complete.

## C.5 Performing Detailed Model Evaluation

The second-tier analysis was a head-to-head comparison of model components that had survived the first-tier screening. As stated earlier, it was not the intent of this study to identify the "best" model for use in any one setting. Hence, the second-tier analysis was not a further screening. Rather, the goal was to document, with considerable detail, a comparison of important modeling features and capabilities for the most promising models in each class of the contaminated sediment modeling system. It is anticipated that this documented comparison will provide a sound basis for selecting the models best suited for numerous research applications carried out at ERD and elsewhere.

The QA/QC component for performing detailed model evaluation was comprised of the following:

- Current documentation and supporting materials for each selected model or model component were obtained.
- A designated Study Team member characterized each selected model component using the established comparison criteria.
- In the event that an evaluator identified a possible improvement or addition to the comparison criteria, the Study Team considered, and either approved or disapproved, the modification of the comparison criteria to accommodate the change.
- In some instances the evaluation of models included personal contact with model developers to verify and expand the Study Team's conclusions.
- The characterization data for all model components were compiled in comparison matrices and supporting text.
- The investigators for the three participating firms reviewed the compiled results for all model components prior to the submittal of the draft final report to the WAM.
- The Study Team responded to questions/comments related to the model comparisons in the WAM's review of the draft final report, and modified the report as appropriate.

C.6 Developing Recommendations

At the conclusion of this study, recommendations and conclusions were developed regarding (1) the most promising models and modeling components that were identified, (2) limitations to the currently available contaminated sediment modeling capabilities, and (3) R & D opportunities for correcting the identified limitations.

C.7 Evaluating Model Linkage Approaches

For this task, the Study Team performed an evaluation of the selected models for possible linkage with comprehensive watershed models such as the Hydrological Simulation Program - FORTRAN (HSPF). The purpose of the evaluation was to ascertain the relative "compatibility" of each model with a model such as HSPF, and to identify potential problems in implementing a linkage. Compatibility issues that were considered included mismatches in model paradigms; irresolvable mismatches between HSPF watershed model outputs and required receiving water model inputs; mismatches in development platform; complications due to differing code architectures; and others. It was necessary and advantageous to perform this evaluation by considering linked systems of contaminated sediment modeling components.

The QA/QC component for evaluating model linkage approaches was comprised of the following:

- An objective and defensible method of deciding which, and how many, linked modeling systems should be evaluated for linkage was defined.
- To the extent possible the results of the linkage evaluations for the selected modeling systems were presented in a comparative format. That is to say, an effort was made to present the results in a format that will enable ERD to draw direct comparisons between the issues involved in linking one model versus another

C.8 Documenting Results

The Study Team provided a report for each of the four study tasks. The first two reports ("Task

1: Develop Evaluation Criteria and "Task 2: Identify Candidate Models") served as preliminary documents to encourage discussions between the EPA WAM and the Study Team, and to assure that the study was proceeding in an appropriate manner to meet the expectations of the EPA and the WAM. The final two reports, combined into a single product, ("Task 3: Perform Comprehensive Model Evaluation" and "Task 4: Evaluate Model Linkage Approaches") will likely have a broader audience, and collectively documented all the important study results. The combined report included a full description of the study methodology, the study results and our recommendations.

The QA/QC component for documenting study results in the final two reports was comprised of the following:

- A clear description of the study methodology was developed, and it was used it to introduce and clarify the results that were presented.
- To provide clarity in documenting the results of model comparisons, the use of comparison matrices was maximized.
- All models were treated in an equal fashion, and made every effort to avoid inadvertently 'skewing' the documentation of the results because of greater personal familiarity with particular models. The deliverables were reviewed to identify and correct any aberrations from this policy.