

Water Contamination Modeling—A Review of the State of the Science

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Received December 2, 2012; revised January 3, 2013; accepted January 12, 2013

ABSTRACT

This paper reports on the current state of surface water and ocean contamination models—based on the needs of US Government agencies, their Information Technology (IT) systems, and business processes. In addition, down-selection and evaluation criteria were applied in a two-step process. In Step 1, sixty five surface water and ocean models were identified and researched. In Step 2, the following criteria were explored for each model: 1) model environment (river, lake estuary, coastal ocean and watershed); 2) degree of analysis (screening model intermediate model, advanced model); 3) availability (public domain, proprietary); 4) temporal variability (steady state or time variable/dynamic); 5) spatial resolution (one, two or three dimensional); 6) processes (flow, transport, both flow and transport in an integrated system); 7) water quality (chemical, biological, radionuclides, sediment); and 8) support (user support/training available, user manuals/documents available).

Keywords: Watershed; Coastal Ocean; Rivers; Modeling; Simulation

1. Introduction

The purpose of this project was to research and report on the current state of surface water and ocean water contamination models. Environmental analysts require estimates of water contamination levels and expected dispersion/transport patterns following intentional or accidental chemical (including crude oil and petroleum products) and radiological releases to aquatic environments. Water contamination modeling assists in assessing potential impacts to human/environmental health and government operations by providing predictive estimates of contaminant concentration, speed and direction of travel. Examples of recent water contamination incidents which are of interest are listed in **Table 1**.

Water quality modeling has evolved significantly in the last century. The period from 1850 to 1930 was the period of scientific and quantitative understanding of the hydrologic cycle and its processes [1]:

- Mulvaney: 1851—Development of concept of time of concentration.
- Darcy: 1856—Established basic law of groundwater motion.
- St. Venant: 1871—Derived the equations of one-dimensional surface water flow.
- Manning: 1891—Developed an equation for open channel flow velocity.
- Green and Ampt: 1911—Development of infiltration

model.

Streeter and Phelps: 1925—Developed the dissolved oxygen sag curve for rivers.

The frequency of these events (**Table 1**) is rare, their impacts are high, and their occurrence is hard to predict. The modeling of the above mentioned events have many associated unknowns. The following characteristics make the event challenging from the modeling perspective.

- Unknown site characteristics—location, soil characteristics, land use, etc.
- Unknown sources of contamination—point or polygon.
- Unknown release rate of contaminants—instantaneous or continuous.
- Unknown deposition rate of contaminants—dry deposit or wet deposit.
- Unknown parameters for data—availability and accessibility of data; sources of data; format of data.

Until the 1960s, the scope of the problems that could be solved was constrained by the computational tools available [2]. The advent of digital computers led to major advances in modeling. Water quality model development and complexity kept pace with the advances in computers. The first advancement in the 1960s was the extension of simple 1-dimensional models to 2-dimensional modeling. This was followed by biological modeling (eutrophication) and then multi-dimensional and multi-species modeling. The period since 1980 has seen

Table 1. Examples of water contamination modeling needs.

Contaminant and Incident Type	Aquatic Environment	Predictions	Implications	Example
Radionuclides leak from reactor	Ocean	Concentrations, locations, surface area, weathering, time factors	Water intakes, swimming, fisheries, shipping, military operations	Fukushima, Japan
Petroleum flow from underwater crude oil well				Deepwater Horizon, Gulf of Mexico
Bauxite ore waste (red mud) spill				Ajka, Hungary
Petroleum from crude oil pipeline	Surface water	Concentrations, locations, time	Water intakes, swimming, fishing	Yellowstone River, MT
Coal ash spill				Kingston Fossil Plant, TN
Benzene spill				Songhua, China

the development of user-friendly, GIS-linked hydrologic, hydraulic and water quality models, and extensive use of these models in a variety of applications.

This report focuses on riverine, estuarine, and coastal ocean water contamination modeling and addresses three major components that are important to government agency consideration for model selection, evaluation and implementation:

- Riverine, estuarine, and/or coastal ocean contaminant model.
- Input data for the model.
- Expertise required to run the model and interpret the results.

2. Information and Data Collection

Our first task was to identify and collect information on surface water and ocean contamination models. Water contamination models are developed by many Federal, State, and local agencies, as well as universities, private companies, and non-government organizations. These models were developed for many purposes and by various methods, with varying levels of detail, accuracy and quality. There are literally hundreds of water quality models available. While the number of models is staggering, the fundamental concepts on which they are based are similar. Water quality models represent the following:

- The hydrodynamic flow fields that drive the movement of the water quality constituents.
- The movement and transformations of the water quality constituents.

The large number of models arises from different combinations of these parameters and assumptions and (often minor) differences in the algorithms used to represent particular processes as follows:

- Model Environment—River, Lake, Estuary, Coastal Ocean and Watershed.
- Degree of Analysis—Models are developed at various levels of complexity, depending on the application needs. The simplest models provide general predic-

tions based on a limited set of environmental or physical factors. The most sophisticated models will solve fundamental equations on a detailed spatial and temporal scale. These models may be integrated with a geographic information system (GIS) which is used to provide spatially-arrayed input data or to spatially display the model results.

- Screening models use empirical model/analytical methods for contaminant transport.
- Intermediate models—These are hybrid models that do not require a rigorous mathematical solution.
- Advanced models—Models that approximate a solution of governing partial differential equations that describe a natural process. The approximation uses a numerical discretization of the space and time components of the system or process. The advanced models use the following solution techniques for solving the system of equations; Finite Difference; Finite Element; Finite Volume; Harmonic Models (best for tidal basins); Methods of Characteristics (Eulerian-Lagrangian Models); Random Walk and Random Flight Particle Tracking.
- Availability—Public Domain, Proprietary, Restricted Support (support only for the developing organization).
- Temporal Variability—Steady State or time variable/dynamic.
 - Steady state model—Mathematical model of fate and transport that uses temporally constant values of input variables to predict constant values of receiving water quality concentrations.
 - Time variable model—A mathematical formulation describing the physical behavior of a system or a process and its temporal variability.
- Spatial Resolution—Models may be one-, two- or three-dimensional. One-dimensional models are the most common type and generally the easiest to use but may not provide sufficient spatial representation in some cases.
 - One-dimensional models are limited to the simu-

lations of cross-sectional averages generally based on the use of the Chezy or Manning equation to specify friction losses and the use of the dispersion coefficient of mixing to quantify mixing. They cannot effectively model steep slopes and stratified exchange of fresh and sea water.

- Two-dimensional models explicitly represent variations in two dimensions. This may be x-y representation with complete mixing in the z-direction, x-z representation with complete mixing in the y-direction (estuaries), or y-z mixing with complete mixing in the x direction. 2-D horizontal plane models simulate estuaries as well mixed vertically. They represent lateral and longitudinal variations in velocity and constituent concentration for estuaries with non-uniform widths. 2-D models explicitly represent variations in two dimensions with the third dimension assumed to be completely mixed.
- Three-dimensional models explicitly represent movement, variations and transformations in x-y-z space.
- Processes—Flow, Contaminant Transport, both Flow and Transport in as an integrated system.
 - Flow model—Calculates hydrology and hydrodynamic conditions (flow, velocity, surface runoff) which are then used as input to a water quality transport model.
 - Transport model—calculates the movement and transformation of water quality constituents.
 - Both—Hydrologic/hydrodynamic and transport models are integrated into a single Model.
- Water Quality—Chemical, Biological, Radionuclides, Sediments.
- Support—User Support/training available, User Manuals/documents available.

3. Model Review Methodology

The model review consisted of a two-step process (model

identification and summarization of capabilities):

Step 1. Model Identification—The search for available models for river and ocean contamination was initiated by literature review. A comprehensive list of models was developed. The review included the following sources:

- USEPA Water Quality model use database.
- USEPA Council for Regulatory Environmental modeling.
- USACE Environmental Laboratory.
- USGS—The Surface Water and Water Quality Models Information Clearinghouse (SMIC).
- Water Environment Research Foundation (WERF).
- UNESCO.
- Ministry of Environment, Parks, and Land (British Columbia, Canada).
- National Council on Radiation Protection and Measurements.
- Open Literature.
- http://www.ncasi.org/programs/areas/water/emrg/werf_aera.htm.
- http://smig.usgs.gov/SMIG/model_archives.html.

Step 2. Summarization—The models were summarized based on the information available from the literature and the criteria presented in **Table 2** below.

The results are shown in **Tables 3** and **4**. **Table 3** provides the acronyms, names, and availability information of the water contamination models that were identified in the literature review. The salient features and functionality of the available models is summarized in **Table 4**.

4. Development of Model Selection Criteria

The proper selection of a model is essential to the successful simulation of water contamination modeling. Model selection is the first step in a modeling task. As shown in **Tables 3** and **4**, there are numerous riverine and ocean water models available. Government requirements can be met with a suite of models appropriate for riverine, estuarine, and the coastal ocean environment.

Table 2. Model selection criteria.

Criteria	Parameters
Model environment	River, lake, estuary, coastal ocean and watershed
Degree of analysis	Screening models, intermediate models, advanced models
Availability	Public domain, proprietary
Temporal variability	Steady state or time variable/dynamic
Spatial resolution	One-, two- or three-dimensional
Processes	Flow, transport, both flow and transport in an integrated system
Water quality	Chemical, biological, radionuclides, sediment
Support	User support/training available, user manuals/documents available

Table 3. Summary table of model names, references and availability.

Acronym	Model Name	Reference	Availability
AQUATOX	Fate and Ecological Effects in Aquatic Ecosystems	[3]	http://water.epa.gov/scitech/datait/models/aquatox/index.cfm
ADCIRC	Advanced Circulation Model for Oceanic, Coastal and Estuarine Waters	[4]	http://www.unc.edu/ims/adcirc/document/ADCIRC_title_page.html http://www.adcirc.org/
Bath tub		[5,6]	http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=watqual
BLTM	Branched Lagrangian Transport Model	[7,8]	http://smig.usgs.gov/cgi-bin/SMIC/model_home_pages/model_home?selection=bltm
BRANCH	Branched-Network Dynamic Flow Model	[9]	http://smig.usgs.gov/cgi-bin/SMIC/model_home_pages/model_home?selection=branch
CAFEX	Circulation Analysis with Finite Element Explicit Method	[10]	http://books.google.com/books?id=tHICGyOoK1oC&pg=PA686&lpg=PA686&dq=CAFEX+circulation&source=bl&ots=S-nSK7nIpw&sig=hhSu0z6W7MRSV4sSGe98zpCzIYM&hl=en#v=onepage&q=CAFEX%20circulation&f=false
CE-QUAL-ICM	2-D (horizontal) and 3-D water quality model	[11]	http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=watqual
CE-QUAL-R1	1-D (vertical) reservoir water quality model	[12]	http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=watqual
CE-QUAL-RIV1	Corps of Engineers-Quality-Rivers	[13]	http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=watqual
CE-QUAL-W2	Corps of Engineers-Quality-2-D	[14, 15]	http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=watqual
CH3D-WES	Curvilinear-Hydrodynamics in Three-Dimensions—Waterways Experiment Station	[16]	http://chl.erdc.usace.army.mil/chl.aspx?p=s&a=Software;22
CHEN's Model	Mathematical Model for Water Quality Analysis	[17]	http://mdl.csa.com/partners/viewrecord.php?requester=gs&collection=ENV&recid=8005190&q=Chen+H.+S.%2C+1978.+A+mathematical+model+for+water+quality+analysis%2C&uid=788372443&setcookie=yes
CMS	Contaminant Model for Streams	[18]	http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=watqual
CORMIX	Cornell Mixing Zone Model (Expert System)	[19]	http://water.epa.gov/scitech/datait/models/cormix.cfm
CTAP	Chemical Transport Analysis Program	[20]	http://books.google.com/books?id=EYPuwIMgBT4C&pg=SA11-PA14&lpg=SA11-PA14&dq=CTAP+Hydroqual&source=bl&ots=iph40_Ya-3&sig=4sNDHw_B-wus1IHgzAd_Xt6lkbc&hl=en#v=onepage&q=CTAP%20Hydroqual&f=false
DAFLOW	Diffusion Analogy form of the FLOW equations	[21]	http://smig.usgs.gov/cgi-bin/SMIC/model_home_pages/model_home?selection=daflow
DEM	Dynamic Estuary Model	[22]	http://sdi.odu.edu/mbin/wasp/dos/dynamic_estuary_model_dynhyd5.pdf
DELFT3D	DELFT 3-D Model	[23]	http://www.deltaressystem.com/hydro/product/621497/delft3d-suite
DR3M	Distributed Routing Rainfall-Runoff Model	[24]	http://smig.usgs.gov/cgi-bin/SMIC/model_home_pages/model_home?selection=dr3m
DYNLET	Dynamic behavior of the tidal flow at inlet	[25]	http://chl.erdc.usace.army.mil/chl.aspx?p=s&a=SOFTWARE;30
ECOM-3D	Estuarine Coastal and Ocean Model	[26,27]	http://www.hydroqual.com/ehst_env_hyd.html
EFDC	Environmental Fluid Dynamics Code	[28]	http://www.epa.gov/ceampubl/swater/efdc/index.html
EHSM3D	Three-Dimensional Estuarine Hydrodynamic Software Model	[29]	http://books.google.com/books?id=GtfEBCUDhHwC&pg=PA171&lpg=PA171&dq=EHSM3D+sheng&source=bl&ots=PqqCbnu4k&sig=l4JrY5gHC1z9cI-dbs8oUNUXXJA&hl=en#v=onepage&q=EHSM3D%20sheng&f=false

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EPA Screening Procedures	Water Quality Screening for Toxic and Conventional Pollutants	[30,31]	http://www.epa.gov/waterscience/library/modeling/wqascreenpart1.pdf http://water.epa.gov/scitech/datait/models/upload/2009_01_13_models_wqascreenpart2.pdf
EXPLORE-1	Quasi 2-D Tidal Flow Model	[32]	http://nepis.epa.gov/Exe/ZyNET.exe/2000HM67.TXT?ZyActionD=ZyDocument&Client=EPA&Index=1981+Thru+1985&Docs=&Query=&Time=&EndTime=&SearchMethod=1&TocRestrict=n&Toc=&TocEntry=&QField=&QFieldYear=&QFieldMonth=&QFieldDay=&IntQFieldOp=0&ExtQFieldOp=0&XmlQuery=&File=D%3A%5Czyfiles%5CIndex%20Data%5C81thru85%5Ctxt%5C00000003%5C2000HM67.txt&User=ANONYMOUS&Password=anonymous&SortMethod=h%7C-&MaximumDocuments=1&FuzzyDegree=0&ImageQuality=r75g8/r75g8/x150y150g16/i425&Display=p%7Cf&DefSeekPage=x&SearchBack=ZyActionL&Back=ZyActionS&BackDesc=Results%20page&MaximumPages=1&ZyEntry=1&SeekPage=x&ZyPURL
FETRA	Finite Element Transport	[33,34]	http://www.osti.gov/bridge/product.biblio.jsp?osti_id=5951347
GEMSS	Generalized Environmental Modeling System for Surface waters-Hydrodynamic Module	[35]	http://www.erm-smg.com/gemss.html
GEOSFM	Geospatial Stream Flow Model	[36]	http://earlywarning.usgs.gov/fews/geosfm.php
GLLVHT	Generalized, Longitudinal-Lateral-Vertical Hydrodynamics and Transport	[37]	http://www.erm-smg.com/gemss.html
GNOME	General NOAA Operational Modeling Environment	[38]	http://response.restoration.noaa.gov/gnome
GSSHA	Gridded Surface Subsurface Hydrologic Analysis	[39]	http://chl.ercd.usace.army.mil/gssha
HEC-HMS	Hydrologic Modeling System	[40]	http://www.hec.usace.army.mil/software/hec-hms/index.html
HEC-RAS	River Analysis System	[41]	http://www.hec.usace.army.mil/software/hec-ras/
HOTDIM	Hydro Dynamics of Three Dimension	[42]	Tennessee Valley Authority
HSCTM2D	Hydrodynamic, Sediment, and Contaminant Transport Model	[43]	http://www.epa.gov/ceampubl/swater/hsctm2d/index.html
HSPF	Hydrological Simulation Program	[44]	http://www.epa.gov/ceampubl/swater/hspf/index.html
ICWater	Incident Command Tool for Drinking Water Protection	[46]	http://eh2o.saic.com/icwater/
John Paul's Model	Water quality model	[47,48]	http://books.google.com/books?id=HICGyOoK1oC&pg=PA709&lpg=PA709&dq=john+paul's+water+quality+model&source=bl&ots=S-nSK7oIvs&sig=7Gk-YxlzZEZ_a7vnP_Eqz0TI-hg&hl=en#v=onepage&q=john%20paul's%20water%20quality%20model&f=false
MECCA	Model for Estuarine and Coastal Circulation Assessment	[49]	http://www.nauticalcharts.noaa.gov/csdl/publications/TR_NOS-CS05_FY00_Hess_MECCA2.pdf
MIKE11	Generalized Modeling Package-1D-Hydrodynamics	[50]	http://www.dhisoftware.com/sitecore/content/Microsites/MIKEbyDHI/Products/WaterResources/MIKE11.aspx
MIKE-21	Generalized Modeling Package-2D-Hydrodynamics	[51]	http://www.dhisoftware.com/sitecore/content/Microsites/MIKEbyDHI/Products/CoastAndSea/MIKE21.aspx
MIKE-3	Generalized Modeling Package-3D-Hydrodynamics	[52]	http://www.dhisoftware.com/sitecore/content/Microsites/MIKEbyDHI/Products/CoastAndSea/MIKE3.aspx
MIKE-SHE	MIKE-Système Hydrologique Européen (SHE)	[53]	http://www.dhisoftware.com/sitecore/content/Microsites/MIKEbyDHI/Products/WaterResources/MIKESHE.aspx
MIT Model	M. I. T. Transient Water Quality Network Model	[54]	http://yosemite.epa.gov/water/owrcatalog.nsf/9da204a4b4406ef885256ae0007a79c7/18af4d194895d1a58525700500662f14!OpenDocument

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NELEUS	Hydrodynamics and transport for water quality	[55-57]	http://books.google.com/books?id=HICGyOoK1oC&pg=PA689&lpg=PA689&dq=NELEUS+water+model&source=bl&ots=S-nSK7oIqx&sig=bUu8JeYmKZ-KyopCX683QJV6sCw&hl=en#v=onepage&q=NELEUS%20water%20model&f=false
OTEQ	One-Dimensional Transport with Equilibrium Chemistry	[58]	http://water.usgs.gov/software/OTEQ/
OTIS	One-Dimensional Transport with Inflow and Storage	[59]	http://water.usgs.gov/software/OTIS/
POM	Princeton Ocean Model	[26,27]	http://www.aos.princeton.edu/WWWPUBLIC/htdocs.pom/
PRMS	Precipitation-Runoff Modeling System	[60]	http://smig.usgs.gov/cgi-bin/SMIC/model_home_pages/model_home?selection=prms
QUAL2K	River and Stream Water Quality Model	[61,62]	http://www.epa.gov/athens/wwqtsc/html/qual2k.html
QWASI	Quantitative Water Air Sediment Interaction Model	[63]	http://www.trentu.ca/academic/aminss/envmodel/models/QWASI310.html
RMA2			http://chl.erdc.usace.army.mil/rma2
RMA10	Resource Management Associates	[64]	http://chl.erdc.usace.army.mil/rma10
RAM4			http://chl.erdc.usace.army.mil/rma4
RECOVERY	A Mathematical Model to Predict the Temporal Response of Surface Water to Contaminated Sediments	[65]	http://el.erdc.usace.army.mil/elmodels/pdf/w-94-4.pdf
RIVMOD-H	River Hydrodynamics Model	[66]	http://books.google.com/books?id=HICGyOoK1oC&pg=PA308&lpg=PA308&dq=RIVMOD-H&source=bl&ots=S-nSK7oKos&sig=RRs3sep3ZMqNunaBvVjXVdNxMiQ&hl=en#v=onepage&q=RIVMOD-H&f=false
ROMS	Regional Ocean Model System	[67]	http://www.myroms.org/
SED-2D	Two-Dimensional, vertically averaged sediment transport	[68]	http://chl.erdc.usace.army.mil/sed2d
SERAFM	Spreadsheet-based Ecological Risk Assessment for the Fate of Mercury	[69]	http://www.epa.gov/ceampubl/swater/serafm/index.html
SEDZL	Sediment Transport and Contaminant Transport Model	[70,71]	www.epa.gov
SERATRA	Sediment Contaminant Transport Model	[34,72]	http://nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=2000HM49.txt
SHARC	System for Hazard Assessment of Released Chemicals	[73]	http://www.asascience.com/asasearch/services/defense/SHARC_Tech-brochure.pdf
SMS	Surface Water Modeling Simulation	[74]	http://chl.erdc.usace.army.mil/sms
SIMSYS2D	Two-dimensional simulation of hydrodynamics and water quality	[75-77]	http://www.rand.org/pubs/papers/P6646.html
SWMM	Storm Water Management Model	[78]	http://www.epa.gov/nrmrl/wswrd/wq/models/swmm/index.htm
TRIM	Tidal, Residual, Intertidal Mudflat	[79]	
WASP	Water Quality Analysis Simulation Program	[80,81]	http://www.epa.gov/athens/wwqtsc/html/wasp.html
WIFM-SAL	WES Implicit Flooding Model-SAL	[82]	http://books.google.com/books/about/User_Guide_for_WIFM_SAL_WES_Implicit_FloX.html?id=FznRNwAACAAJ
WQMAP	Water Quality Mapping and Analysis Package	[83]	http://asascience.com/software/wqmap/index.shtml

Table 4. Comparative features and functionality of water contamination models.

Model	Model Environment				Degree of Analysis			Availability		Temporal Variability		Spatial Resolution			Processes		Water Quality			Support				
	River	Lake	Estuary	Coastal Ocean	Watershed	Screening	Intermediate	Advanced	Public	Proprietary	Restricted Support	Steady State	Time Variable	1-D	2-D	3-D	Flow Model	Transport Model	Both	Chemical	Biological	Radionuclide	Sediment	User Support Availability
AQUATOX	✓	✓				✓			✓			✓	✓	✓				✓	✓	✓				✓
ADCIRC	✓		✓	✓		✓		✓	✓			✓	✓		✓	✓	✓							✓
Bathtub		✓				✓			✓			✓						✓		✓				✓
BLTM	✓		✓						✓					✓				✓		✓				✓
BRANCH	✓	✓	✓			✓			✓			✓	✓				✓			✓				✓
CAFEX			✓	✓				✓		✓		✓			✓			✓	✓					✓
CE-QUAL-ICM	✓	✓	✓						✓		✓	✓	✓	✓	✓	✓		✓		✓	✓		✓	✓
CE-QUAL-R1		✓							✓		✓	✓	✓	✓				✓		✓	✓		✓	✓
CE-QUAL-RIV1	✓					✓			✓		✓	✓	✓					✓		✓	✓		✓	✓
CE-QUAL-W2	✓		✓			✓			✓		✓	✓	✓		✓			✓	✓	✓		✓		✓
CH3D-WES	✓	✓	✓			✓			✓		✓	✓	✓			✓		✓	✓					✓
CHEN's Model	✓		✓	✓				✓		✓		✓			✓			✓	✓					✓
CMS	✓					✓			✓			✓						✓	✓	✓				✓
CTAP	✓					✓				✓		✓						✓						✓
DAFLOW	✓								✓					✓				✓						✓
DEM			✓			✓			✓			✓						✓	✓					✓
DELFT3D	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓	✓	✓	✓	✓
DR3M					✓		✓		✓			✓			✓			✓						✓
DYNLET	✓		✓	✓				✓	✓			✓	✓					✓						✓
ECOM-3D			✓	✓				✓		✓		✓	✓	✓	✓	✓		✓						✓
EFDC	✓	✓	✓						✓			✓	✓	✓	✓	✓		✓	✓	✓		✓		✓
EHSM3D		✓	✓					✓	✓			✓			✓			✓	✓					✓
EPA Screening Procedures	✓	✓	✓			✓			✓			✓	✓	✓	✓	✓		✓	✓	✓	✓	✓	✓	✓
EXPLORE-1	✓					✓				✓		✓			✓			✓		✓	✓			✓
FETRA			✓					✓	✓			✓			✓			✓			✓	✓		✓
GEMSS	✓	✓	✓	✓		✓	✓		✓			✓	✓	✓	✓	✓		✓	✓	✓		✓		✓
GEOFSM	✓						✓		✓			✓	✓					✓						✓
GNOME			✓	✓			✓		✓			✓	✓					✓		✓				✓
GSSHA	✓							✓	✓			✓			✓			✓						✓

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HEC-HMS			✓		✓	✓	✓		✓			✓	✓
HEC-RAS	✓				✓	✓	✓	✓	✓			✓	✓
HOTDIM		✓			✓	✓			✓		✓	✓	✓
HSCTM2D		✓	✓		✓	✓		✓	✓		✓	✓	✓
HSPF			✓		✓						✓	✓	✓
ICWater	✓			✓	✓		✓	✓		✓	✓	✓	✓
John Paul's Model		✓	✓		✓	✓		✓	✓	✓	✓		
MECCA	✓	✓	✓	✓	✓	✓		✓	✓		✓	✓	✓
MIKE11	✓	✓		✓	✓	✓	✓	✓			✓	✓	✓
MIKE-21		✓	✓	✓	✓	✓	✓		✓		✓	✓	✓
MIKE-3	✓	✓	✓	✓	✓	✓	✓		✓		✓	✓	✓
MIKE-SHE			✓		✓	✓	✓				✓		✓
MIT Model		✓			✓	✓		✓	✓		✓	✓	✓
NELEUS		✓			✓	✓		✓	✓		✓	✓	✓
OTEQ	✓				✓	✓		✓	✓		✓	✓	✓
OTIS	✓				✓	✓		✓	✓		✓	✓	✓
PRMS			✓	✓	✓		✓	✓		✓		✓	✓
QUAL2K	✓				✓	✓		✓	✓		✓	✓	✓
QWASI					✓	✓				✓		✓	✓
RMA2	✓	✓	✓		✓	✓	✓	✓	✓	✓		✓	✓
RMA10	✓	✓	✓		✓	✓	✓	✓		✓		✓	✓
RAM4	✓	✓	✓		✓	✓	✓	✓	✓	✓		✓	✓
RECOVERY	✓				✓	✓		✓	✓		✓	✓	✓
RIVMOD-H	✓			✓	✓	✓	✓	✓		✓		✓	✓
ROMS			✓		✓	✓		✓			✓	✓	✓
SED-2D	✓	✓	✓		✓	✓	✓		✓		✓	✓	✓
SEDZL	✓		✓		✓	✓		✓	✓		✓	✓	✓
SERATRA	✓				✓	✓		✓	✓		✓	✓	✓
SHARC			✓	✓	✓	✓		✓		✓	✓	✓	✓
SMS	✓	✓	✓		✓						✓		✓
SIMSYS2D			✓	✓	✓	✓		✓	✓		✓	✓	
SWMM	✓				✓	✓		✓	✓		✓	✓	✓
TRIM			✓	✓	✓	✓		✓	✓	✓		✓	✓
WASP	✓	✓	✓		✓	✓		✓	✓	✓	✓	✓	✓
WIFM-SAL			✓		✓	✓		✓	✓		✓	✓	✓
WQMAP	✓				✓	✓		✓		✓	✓	✓	✓

The selection of these models is based on meeting a specific modeling objective (e.g., a toxic spill in a river affecting drinking water supplies downstream).

The major differentiators between the models identified in this report is the way they handle spatial and temporal dimensions and how they model the fate and transport processes. Not all models, however, are appropriate under all conditions. They vary greatly with respect to their analytical approach, underlying assumptions, data needs, and output capacity. The process of selecting a model is not limited to evaluating the model science. The level of sophistication required in a modeling study reflects constraints such as:

- Accuracy required.
- Allotted time frames for study completion.
- Availability and reliability of input data.
- Training and expertise required for model operation.

These constraints and others combine to determine whether modeling is an appropriate tool for achieving the objectives, which model is the best choice for application and the limitations in interpreting the model results. Confidence in model results is based on the quality of data used to construct the model, the capabilities of the modeler, and the proven ability of the model to simulate observed phenomena [84]. For the development of the model selection criteria, issues addressed by the National Research Council [85], Environmental Protection Agency [86] and criteria discussed in the literature were reviewed. The following three issues were addressed in developing the model selection criteria:

- Model characteristics.
- Input data.
- Technical expertise.

4.1. Model Characteristics

The choice of the appropriate level of model complexity is determined in large measure by the nature of problem. The ability to model the transport, transformation and fate of sediments and interacting contaminants in surface water systems rests upon the ability to select a model or models which appropriately represents the most significant processes controlling the system. Since model studies are most often conducted under economically imposed constraints, including personnel, model software availability, computer hardware limitations, and the availability of field data for model calibration and validation, modeling strategies often necessitate selection of a model which meets minimum, but acceptable, criteria for process representation. The model selection criteria are organized into three categories as described below:

Application criteria specify the nature and intent of the analysis to be performed. The application criteria for model selection are based primarily on:

- Consistency of the model with the scientific theory.
- Model appropriateness for the complexity of the problem.
- Identification of the problem.
- Relationship of the model to the problem.
- Availability in public domain.

Technical criteria specify the site-specific processes to be simulated by the model. The technical criteria for model selection are based primarily on:

- Physical mixing and transport processes.
- Biological, chemical, and physical degradation and transformation processes.
- Geometry and/or dimensionality and time variability of the system.
- Temporal and spatial scales and extent of the models.
- Content, accuracy, currency and resolution of data available for modeling.
- Quantification of the uncertainty.
- Model is consistent with the amount of data available.
- Solution scheme examination.
- Model calibration and validation.
- Compatibility with Geographic Information System (GIS).
- Ease of output comprehension (e.g. graphs, maps, etc.).

Operational criteria specify the quality assurance (QA) and documentation requirements. The operational criteria are related to the degree of quality assurance (QA) and documentation to which a model has been subjected.

- Availability of test problems for comparison either in the user's manual or from the source where the model was obtained.
- Proven track record for the model—model must have been applied and calibrated to real world problems rather than have been developed and applied in theoretical hypothesis testing.
- Flexible for future updates and improvements.
- Cost for annual model support is an acceptable long-term expense.

4.2. Input Data to Support the Model

The model data plays a crucial role in the model selection process. For water contamination modeling, three types of data are required.

- Input data.
- Data for calibrating the model.
- Data for validating the results.

Issues pertaining to assembling and entering data into the model include the following:

- Existence of data.
- Collection of data (data collection is a resource intensive exercise which can be a critical factor during emergencies).

- Availability of data (public vs. proprietary; classified vs. unclassified).
- Accessibility of data (hardcopy vs. electronic).
- Format of the data (pre-processing of data in model compatible format).

4.3. Expertise of the Modeler

A typical modeling application requires data collection, data preparation, model simulations, results interpretation, and model reporting. All these steps are dependent on the expertise of the modeler. Expertise of the modeler will have a major impact on model results.

Staff resources are also a major consideration in modeling. Familiarity of the modeler with a particular type of model (e.g., finite element versus finite difference), or direct experience with a model sometimes get considered as a factor in the model selection. But in no case, however, should familiarity with a model dictate its selection when it does not satisfy the objective, technical, and implementation criteria.

5. Summary and Conclusions

5.1. Model Evaluation Criteria

Modeling strategies often necessitate selection of a model which meets minimum but acceptable evaluation criteria. The current model evaluation criteria are based on the information collected and analyzed. The evaluation criteria include the following:

Application Evaluation for model selection consists of the following parameters:

- Model/software availability and cost.
- Computer hardware limitations.
- Methods—Modeling approaches for the major processes flow, chemical fate and transport processes.
- Output—Type of outputs and output options, Level of outputs.
- User Interface—Input helpers, windows based or raw edits of input files, GIS interface for data.

Technical Evaluation for the model selection includes the following parameters:

- Model Environment—River, lake, estuary, ocean, watershed.
- Degree of Analysis—Screening, intermediate, advanced.
- Availability—Public, proprietary.
- Type—Steady state, dynamic.
- Level of Complexity—1-D, 2-D, 3-D.
- Processes—Flow, transport, both.
- Water Quality—Chemical, biological, radiological, sediment.
- Scale—Spatial, temporal.
- Input data required for model simulation, calibration

and validation.

- Data—Data requirements and sources, level of accuracy of the data.

Operational Evaluation for the model selection includes the following parameters:

- Supporting Materials—Example input and output data sets, Identification of sensitive input parameters, calibration procedures for field measurements, continuing education and training.
- Availability and user friendliness of the interface for ease of input preparation.
- GIS linkage—for large modeled areas.
- Model Availability—Model contacts, documentation, source availability, version tracking.

5.2. Data as Evaluation Criteria

For Outside the Continental United States (OCONUS) riverine, estuarine, and ocean modeling applications, data can be a limiting factor.

- Availability of data in foreign countries can be a limiting factor, especially in regions of conflict. For example, no hydrological data has been collected in Afghanistan after 1979.
- Collection and preparation of data even for a simple model requires time. This is particularly important in emergency situations where fate and transport of contaminants is required immediately for a proper response. Therefore, focus on data should also be an important factor in model selection.
- Language is a major barrier for data collection in foreign countries. Usually countries collect data in their national language and rarely is it available online or translated into the English language.
- Data may be collected only for the main reaches of major rivers or estuaries. Data for other hydrological parameters (depth, width, velocity, roughness coefficients etc.) may not be available.
- In many developing countries data is not freely available. In many countries because of unresolved transboundary issues data is not freely distributed.
- In developing countries hydrologic data is more available than water quality data because of resource development and management.

5.3. Technical Expertise as Evaluation Criteria

Technical expertise of the modeler should be considered as part of the evaluation criteria. The modeler is the human interface in the whole modeling exercise. The modeler not only runs the model but also calibrates the model, validates the results, and interprets the output. The following criteria should be considered for the technical expertise evaluation:

- Level of technical expertise needed to run the selected model.
- Manpower required to run the model.
- Training requirements.
- IT support for the model.

5.4. Additional Criteria

A critical requirement of several government agencies is to acquire the capability to model “unusual events” in the aquatic environment. These “unusual events” have certain modeling and data unknowns as illustrated below. These unknowns are the limiting factors for model selection.

- Site characteristics.
- Sources of contamination—point, polygon, instantaneous, continuous.
- Release rate of contaminants.
- Deposition rate of contaminants.
- Data.
 - Availability and accessibility of data.
 - Sources of data.
 - Format of data.

6. Acknowledgements

The authors wish to thank Dr. Alan Blumberg and Dr. Walter Grayman for their comments, reviews and suggestions regarding this study.

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