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Selection Criteria for Mathematical Models Used in Exposure Assessments

Surface Water Models

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SELECTION CRITERIA FOR MATHEMATICAL MODELS USED IN EXPOSURE ASSESSMENTS: SURFACE WATER MODELS

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CONTENTS

Tables v
Figures. vi
Foreword vii
Preface. viii
Abstract ix
Authors, Contributors, and Reviewers x

1. INTRODUCTION. 1-1

1.1. ESTIMATING EXPOSURE AREAS. 1-1
1.2. MODEL SELECTION PROCESS. 1-3
1.3. DOCUMENT OBJECTIVES. 1-3

2. BACKGROUND INFORMATION. 2-1

2.1. DEFINITION OF TERMS. 2-2
2.2. BASIC MATHEMATICAL MODEL EQUATIONS 2-6
2.3. HYDROLOGIC TRANSPORT PROCESSES 2-9
2.4. ATTENUATION MECHANISMS 2-11

2.4.1. Hydrolysis. 2-13
2.4.2. Oxidation-reduction 2-13
2.4.3. Photolysis. 2-14
2.4.4. Volatilization. 2-14
2.4.5. Sorption. 2-15
2.4.6. Biodegradation. 2-15
2.4.7. Ionization. 2-16

3. MODEL STRUCTURE 3-1

3.1. RIVERS 3-2
3.2. LAKES AND RESERVOIRS 3-7
3.3. ESTUARIES. 3-9
3.4. TEMPORAL SCALE 3-16
3.5. DIMENSIONALITY 3-21
3.6. DEGRADATION PROCESSES. 3-23
3.7. SEDIMENT TRANSPORT AND SORPTION PROCESSES. 3-25
3.8. NONPOINT SOURCE RUNOFF 3-27

3.8.1. Simple Pollutant Yield Models 3-28
3.8.2. Empirical Loading Functions 3-29
3.8.3. Nonpoint Source Simulation Models 3-30

4. IDENTIFICATION OF MODEL PROCESSES 4-1

4.1. TRANSPORT PROCESSES. 4-3
4.2. DEGRADATION PROCESSES. 4-6

CONTENTS (continued)

5. MODEL SELECTION CRITERIA. 5-1

5.1. STRUCTURE OF THE MODEL SELECTION CRITERIA. 5-4
5.2. MODEL SELECTION PROCESS. 5-7
5.3. DIFFERENT APPLICATIONS 5-26
5.4. MODEL SUMMARY TABLES 5-28

6. USE OF THE SELECTION CRITERIA 6-1

6.1. DESCRIPTION OF EXPOSURE ANALYSIS PROBLEM 6-1
6.2. PRELIMINARY EXPOSURE ASSESSMENT. 6-2

6.2.1. Initial Analysis. 6-2
6.2.2. Selection of a Nonpoint Source Runoff Model . . . 6-3
6.2.3. Surface Water Flow. 6-4
6.2.4. Surface Water Contaminant Transport 6-4

6.3. DETAILED SITE-SPECIFIC ANALYSIS. 6-8

6.3.1. Selection of a Nonpoint Source Runoff Model . . . 6-9
6.3.2. Surface Water Flow. 6-9
6.3.3. Surface Water Contaminant Transport 6-10

7. REFERENCES. 7-1

8. REVIEW OF EXAMPLE SURFACE WATER MODELS. 8-1

8.1. NONPOINT SOURCE RUNOFF MODELS. 8-1
8.2. SURFACE WATER FLOW MODELS. 8-13
8.3. SURFACE WATER TRANSPORT MODELS 8-31

APPENDIX A: DEFINITION OF SYMBOLS A-1

TABLES

3-1 Factors affecting temporal scale. 3-16

5-1 Outline of the model selection process. 5-8

5-2 Summary matrix of nonpoint source runoff models 5-13

5-3 Summary matrix of surface water flow models 5-19

5-4 Summary matrix of surface water contaminant transport models. 5-25

FIGURES

2-1 Block diagram for a water quality system. 2-1

3-1 Vertical representation of a lake and longitudinal representation of a river 3-2

3-2 Ratio of boundary concentration to centerline concentration as a function of dimensionless downstream distance. 3-5

3-1 Classification of estuarine stratification. 3-11

FOREWORD

When performing exposure assessments using predictive methods, assessors frequently ask the following questions: "How do I select the best fate model to use in my assessment," "How can I tell if the model someone else used in their assessment is appropriate," and "What are the strengths and weaknesses of these models?" This document is a first step in addressing these questions.

One of the functions of the Exposure Assessment Group is to develop guidelines for exposure assessments. On September 24, 1986, the U.S. Environmental Protection Agency published Guidelines for Estimating Exposures. During the development of the guidelines and subsequent review and comment, four areas were identified that required further research. One of these areas was selection criteria for mathematical models. This first selection criteria document deals with surface water models. Similar documents will follow dealing with ground-water models and air models, and in the future, other types of models.

This document is designed to help the exposure assessor evaluate the appropriateness of models for various situations. The report defines the terms and discusses the general approaches that modelers take to a problem so that exposure assessors may more readily evaluate the appropriateness of both new and existing models. In addition, step-by-step criteria are provided to enable the assessor to answer the questions posed above. These criteria will eventually be made available as an interactive program for a personal computer (PC).

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PREFACE

The Exposure Assessment Group (EAG) of the Office of Health and Environmental Assessment (OHEA) is preparing several documents addressing selection criteria for mathematical models used in exposure assessments. These documents will serve as technical support documents for the Guidelines for Estimating Exposures, one of five risk assessment guidelines published by the U.S. Environmental Protection Agency in 1986.

The purpose of this document is to present criteria which provide a means for selecting the most appropriate mathematical model(s) for conducting an exposure assessment related to surface water contamination.

The literature search to support the models discussed in this report is current to January 1987.

ABSTRACT

Prior to the issuance of the Guidelines for Estimating Exposures in 1986, the U.S. Environmental Protection Agency (EPA) published proposed guidelines in the Federal Register for public review and comment. The purpose of the guidelines is to provide a general approach and framework for carrying out human and nonhuman exposure assessments for specific pollutants. As a result of the review process, four areas were identified that required further research. One of these was the area of selection criteria for mathematical models used in exposure assessment.

The purpose of this document is to present criteria which provide a means for selecting the most appropriate mathematical model(s) for conducting an exposure assessment related to surface water contamination.

A concerted effort was made to provide general background information regarding surface water flow and contaminant transport and to characterize the important assumptions and limitations of existing models. These include a detailed summary matrix and model writeups for ten runoff models, twelve surface water flow models, and twelve contaminant transport models that have been used previously by EPA to study surface water quality problems. General guidelines and principles for model selection are presented, such as the overview of the modeling process and important issues related to model selection (e.g., familiarity, model reliability, model selection vs. model application). Following the general guidelines is a step-by-step approach for identifying the appropriate model(s) to use in a specific application.

AUTHORS, CONTRIBUTORS, AND REVIEWERS

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1. INTRODUCTION

In the last three decades there has been a dramatic increase in the production and use of chemicals in our society. The chemicals have been developed and applied to a variety of beneficial uses in domestic, industrial, and agricultural applications. In some cases the chemicals have had unexpected adverse effects. As a result, concern has grown over the impacts of some chemicals, both at the point of use or application and in distant areas to which the chemicals may be transported via various environmental pathways.

As the process of regulating and controlling the release of these potentially hazardous chemicals into the environment becomes a more complex task, the U.S. Environmental Protection Agency (EPA) has focused its energy towards a risk assessment/risk reduction framework for making regulatory decisions. Part of this risk assessment process has been the development and publication of the Guidelines for Estimating Exposures (U.S. EPA, 1986). These guidelines "provide the Agency with a general approach and framework for carrying out human or nonhuman exposure assessments for specified pollutants."

1.1. ESTIMATING EXPOSURE AREAS

The five major areas to be evaluated when estimating exposures to environmental contaminants are (U.S. EPA, 1986):

1. Source Assessment -- A characterization of a source of contamination;
2. Pathways and Fate Analysis -- Description of how a contaminant may be transported from the source to the potentially exposed population;
3. Estimation of Environmental Concentration -- An estimate using monitoring data and/or modeling of contaminant levels away from one source where the potentially exposed population is located;
4. Population Analysis -- A description of the size, location, and habits of potentially exposed human and environmental receptors; and

5. Integrated Exposure Analysis -- The calculation of exposure levels and the evaluation of uncertainty.

The process of estimating the environmental concentration of a contaminant plays a significant role in exposure assessment. Often the most critical element is the estimation of a pollutant concentration at an exposure point. This estimation is usually carried out by means of a combination of field data and mathematical modeling results. In the absence of field sampling data, this process relies primarily on the results of mathematical models.

An ideal exposure assessment model would account for multiple emission sources, estimate contaminant concentrations in all media (air, water, food, and soil) resulting from emissions, define multiple pathways of exposure, and estimate exposure to humans, plants, and animals. An ideal model would also contain methods for estimating the simultaneous exposure of humans, plants, and animals to a number of contaminants so that synergistic or antagonistic effects could be estimated as part of a risk assessment. Although the ideal model is not available, component models that address various aspects of exposure assessment are available. Therefore, decisions based on a modeling analysis may require the use of multiple models to account for pollutant transport through different media.

This potential need for multiple model usage in exposure assessments was a major issue during the development of the exposure assessment guidelines.

Prior to the issuance of the Guidelines for Estimating Exposures in 1986, the U.S. Environmental Protection Agency (EPA) published proposed guidelines in the Federal Register for public review and comment. The purpose of the guidelines is to provide a general approach and framework for carrying out human and nonhuman exposure assessments for specific pollutants. As a result of the review process, four areas were identified that required further research. One

of these was the area of selection criteria for mathematical models used in exposure assessment.

1.2. MODEL SELECTION PROCESS

In general, the selection guidelines for mathematical models are written for the exposure assessor, whose goal is to understand the implications that the use of a mathematical model has for exposure assessment. Once this goal is achieved, the assessor can then determine which model(s) best describe the problem that needs to resolved.

Estimating environmental concentrations requires not only the appropriate mathematical model and the necessary data (model input parameter data and field data to compare against the model results), but also the expertise of the exposure assessor. To the extent that the assessment is weak in any of these three areas, the uncertainty in the model results will increase.

1.3. DOCUMENT OBJECTIVES

The purpose of this document is to describe a set of criteria that will assist in the selection of appropriate surface water models suitable for various situations. It is intended primarily to assist potential model users who are not experts in water quality modeling; specifically, to make the reader aware of the complex nature of mathematical modeling, the process involved in choosing a model, and the principles behind the selection.

This document deals with surface water models used to predict pollutant concentrations in water bodies or sediments for nonpoint source runoff, lakes, reservoirs, rivers, and estuaries. The results of these models may be used as input to other models which calculate the dose and associated risk of chemicals to a specific target organism or population.

All of the surface water models presented herein are designed for situations in which the contaminant is at trace concentration levels. A number of

assumptions are implicit in this restriction, including the formulation of the kinetic reactions and the implication that the properties of the contaminant do not affect the properties of the environmental system. The models are not designed to be used in an emergency response framework, such as an accidental spill, because in those situations the contaminant is not likely to be at trace concentrations initially, and the time required to set up the model, run the model, and evaluate results is generally greater than the emergency response times. There are models available to deal with these types of problems; however, they are outside the scope of this report.

Characterizations of the important assumptions and limitations of the existing models are presented in this document, as are definitions of relevant terms. The existing models are generally the best available technology, and are useful tools when applied properly. However, model accuracy is very sensitive to input parameters, and calibration with field data is essential. In any modeling study, the assumptions and limitations of a particular model, along with the means by which it is applied, should be clearly understood by the model user as well as by persons making decisions based, in part, on the modeling results.

The organization of this document is as follows:

Chapter 2. Background Information; definition of terms and descriptions of equations and processes

Chapter 3. Model Structure; descriptions of different water bodies, associated processes, and model formulation

Chapter 4. Identification of Important Processes; simplified analytical means for comparing the relative importance of processes

Chapter 5. Model Selection Criteria; step-by-step process for identifying suitable models

Chapter 6. Use of Selection Criteria

Chapter 7. References

Chapter 8. Review of Example Surface Water Models

2. BACKGROUND INFORMATION

In the exposure assessment field, many of the assessors involved in either the development or review of documents containing modeling results do not necessarily understand the mathematical equations that influence model values. The purpose of this chapter is not to make the reader an "instant" expert in surface water models (modelers themselves have a difficult problem gaining that title), but instead to give the reader a basic understanding of the theory that underlines the modeling process.

Before discussing the basic mathematical equations that make up the model, it is first important to understand the fundamental processes involved in formulating a water quality problem in terms of equations. Thomann (1972) discusses this water quality problem in terms of a system component that identifies those phenomena that are "causation," those that are "responsive," and those that act as links between cause and effect. Figure 2-1 aids in understanding these components for a particular problem.

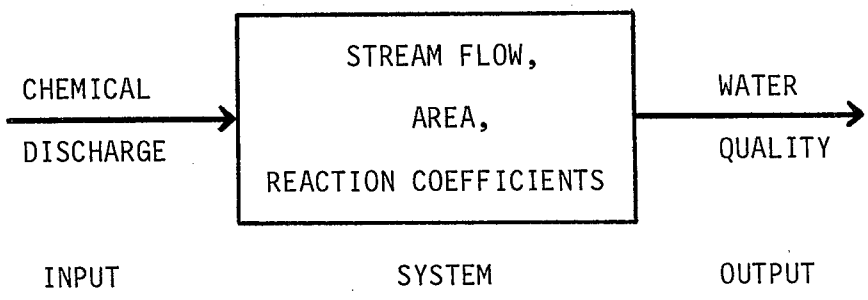

Figure 2-1. Block diagram for a water quality system.

2.1. DEFINITION OF TERMS

Throughout this report, a number of terms or phrases are used which may be interpreted as having somewhat different meanings by readers with varying backgrounds and experience. In an attempt to avoid misinterpretations, this section provides definitions of the following terms: calibration, validation, analytical model, numerical model, mathematical model, screening-level and detail-level assessment, and near-field and far-field analysis.

Calibration -- In this document we will use the term calibration to describe the initial phase of a modeling study, in which the input coefficients of a model are adjusted in an attempt to match measured field data (e.g., velocity, concentration). Model coefficients will differ depending on the types of models being used (nonpoint source, surface water flow, and transport). For example, the types of coefficients that are commonly adjusted in transport models include dispersion coefficients, rate constants, and possibly source and sink terms.

Validation -- This term will be used to describe a separate step of a modeling study where the calibrated model (i.e., fixed coefficients, no further adjustments) is applied to a different set of field data. The validation phase is an attempt to see if the model can reproduce field data under conditions different from those used in the calibration phase. In actual applications, it may be impossible to obtain a separate data set. The calibration phase may also indicate poor model performance and may require that data normally used in the validation phase be used instead to correct the calibrated model. If these circumstances were to occur, the uncertainty in the model results would need to be considered in the decision-making process.

Analytical Models -- Analytical models can usually be represented as models with (1) one or several algebraic equations, (2) one ordinary differen-

tial equation, or (3) one partial differential equation. If a model contains equations which do not fit one of the three classifications given above, the model will usually be difficult to solve by analytical methods (Rich, 1973). An example of an analytical model is the Water Quality Analysis Model (WQAM) by Mills et al. (1982). The WQAM was developed as a computer program to analytically compute surface water concentrations of a chemical in large basins. Solutions of analytical models are exact.

Numerical Models -- Numerical models are usually classified as models with complex mathematical equations that are essentially impossible to solve by analytical methods. Numerical models are written as computer programs because of the complexity of the mathematical equations involved. For example, the WASTOX model (Connolly and Winfield, 1984) is a numerical model for simulating the transport and degradation of toxic chemicals in water bodies, and uses a large number of differential equations to describe the physical system.

The relationship between the analytical and numerical model may be thought of as follows: An analytical solution solves a very simple water quality equation exactly by means of hand calculations. An analytical model solves a more complex, but still relatively simple, set of equations exactly by means of a computer program. A numerical model solves a simple or complex set of equations approximately by means of a computer program.

The terms "analytical code" or "numerical code" typically refer to the computer program (the set of computer instructions written in a programming language and run on a computer), whereas an analytical or numerical model is the implementation of the code with a specific data set (either site-specific or generic) to test the simulated representation of the system against observed or measured behavior.

Mathematical Model -- This term will be used to describe the mathematical representation of the physical system. The model may represent an analytical solution to these equations, or may be an approximate numerical representation of the equations. In some cases, models based on analytical solutions are simple enough that the calculations can be performed using a hand calculator. In other cases the analytical models are more complex, and often are implemented as programs to be run on a computer. In most cases, numerical models are written in a computer language as a program to be run on a computer. Models run on a computer are usually referred to as codes, or computer codes. This document uses the term "model," as opposed to "code" wherever appropriate.

Screening-Level and Detailed-Level Assessment -- The types of modeling analysis that are described in this document may be very broadly categorized as screening-level or site-specific exposure assessment studies. We have chosen to use the term "screening-level" to represent studies where limited calibration and validation data are available and the uncertainty associated with the predicted results is comparatively large, somewhere in the nature of an order of magnitude. The terms "detailed-level" or "site-specific" with regard to analysis are used to predict results on the order of a factor of two to ten. Calibration and validation data are necessary in order to reduce the uncertainty inherent in the results, and also in order to attempt to quantify the bounds of uncertainty associated with the model results in the validation step and with the model results when various model parameters are tested (the latter is called sensitivity analysis).

The models used in a screening-level analysis are generally easier to set up because the analysis requires only a general estimate of the contamina-

tion problem. Models that are used in screening-level analysis make certain restrictive assumptions (loading, stream flow, and time changes are assumed to be constant), so that the results the model generates should reflect these assumptions.

In a more complex site-specific-level analysis, the models used need to account for more random changes in the study area, and are therefore more difficult to use, since the assumptions in the model are not restrictive. In site-specific cases, the input data requirements for the model, i.e., the collection of additional parameter values, are usually substantially greater than in screening-level cases.

Near Field and Far Field -- The mixing of a contaminant in a water body is often separated into two zones, referred to as the near field and the far field. The near field refers to the mixing zone where the properties of the discharged fluid have a significant impact on the mixing and resulting dilution of the discharged fluid by the ambient water body. The important properties of the discharged fluid include the density relative to the ambient water body, and the initial momentum of the discharge. Other characteristics of a discharge pipe, such as a sewage outfall, may be important, and in many cases are designed to maximize the dilution that occurs in the near field. The near-field zone considers the mixing of the initial jet and resulting plume as the discharge is diluted.

The second mixing zone, the far field, refers to the area where the mixing processes are no longer a function of the type of discharge and initial properties of the discharged fluid. In the far field, the mixing processes are dominated by turbulence within the ambient water body and variability of the advective velocity field. All of the models described in this report are intended for the analysis of far-field mixing processes. Detailed descriptions

of the near-field mixing processes, along with descriptions of modeling techniques suitable in this zone, are given by Fischer et al. (1979).

2.2. BASIC MATHEMATICAL MODEL EQUATIONS

Fundamental to the analysis of any water quality problem is the basic equation of continuity, which attempts to describe the relationship of mass transport through a volume of water and the sources and sinks of mass within it. This equation is developed by constructing a material balance about a volume and introducing the principle of the conservation of mass: the time rate of change of mass within the volume plus the net rate of mass flow in and out of the volume must equal that produced by the sources and reduced by the sinks. The continuity equation is a mathematical statement of the principle of mass balance.

All water quality models are based on the conservation of mass. The conservation of mass for the transport of a dissolved contaminant in a water body may be written in differential form as:

$$\frac{\partial C}{\partial t} + \nabla(C\bar{q}) = D\nabla^2 C + \Sigma T + \Sigma r \pm s \qquad \text{(Eq. 2-1)}$$

where

C is the concentration of dissolved contaminant (M/L^3),

t is time (T),

∇ is the Del operator ($\nabla C = \partial C/\partial x + \partial C/\partial y + \partial C/\partial z$) ($1/L$),

$\bar{q}$ is a vector of the x,y,z velocity components (L/T),

D is a dispersion coefficient (L^2/T),

ΣT represents any phase transfer mechanisms ($M/L^3/T$),

Σr represents any reactions ($M/L^3/T$), and

s represents any source or sink terms ($M/L^3/T$).

The statement of the conservation of mass shown in Equation 2-1, also known as the advective dispersion equation, is the fundamental equation in many water quality models. This equation states that the time ratio (t) of change of the substance (c) is equal to the amount of input less both the amount discharged and the amount lost by the decay of the substance in the water body. Generally the advective and dispersive terms, $\nabla(Cq)$ and $D\nabla^2C$, are considered to be the hydrologic or hydrodynamic transport terms, whereas the transfer, reaction, and source/sink terms, ΣT, Σr, and s, are used to represent transformation and degradation processes along with source/sink terms. The source/sink term is usually composed of several components including: (1) point sources, such as a pipe discharge; (2) distributed nonpoint sources, such as runoff along the length of a river; and (3) a distributed source or sink along boundaries of the water body resulting from some previous impact, as in benthal deposits.

One distinguishing characteristic of many toxic substances is their affinity for contaminant adsorption to particulates. As a result, the mass of contaminants is partitioned between the dissolved and the particulate adsorbed forms. In order to develop a descriptive model, two relationships or equations in addition to Equation 2-1 are necessary. The first equation defines the concentration of particulates in the water body, while the second defines a relationship between dissolved contaminants and the contaminants adsorbed to the particulates. The particulate concentration in the water column is generally represented by some form of an advection dispersion equation with the addition of one or more terms, such as a settling velocity acting in the vertical direction. For example:

$$\frac{\partial M}{\partial t} + \nabla(Mq) - w_s \frac{\partial M}{\partial z} = D \nabla^2 M \pm s_m \qquad \text{(Eq. 2-2)}$$

where

M is the concentration of particulate matter (M/L^3),

w_s represents the settling velocity of the particulate (L/T), and

s_m represents any source or sink terms for the particulate ($M/L^3/T$).

The settling velocity used in Equation 2-2 is dependent on the size of the particulate matter, and is usually estimated from basic fluid mechanics principles relating the settling velocity to the diameter and density of the particulate. Under steady-state conditions (when input data such as loading, water flow, velocity, and reaction coefficients are constant over time), Equation 2-2 may be simplified to yield analytical descriptions of the vertical distribution of suspended particulate matter (for examples see Vanoni, 1975). The boundary conditions for the general form of Equation 2-2 are complex relationships relating the erosion and deposition of sediments to the suspended particulate concentration and characteristics of the flow regime in the vicinity of the boundary.

The relationship between dissolved and adsorbed forms of a contaminant is usually represented in the form of an equilibrium partition coefficient. The partition coefficient is defined as the ratio of the mass of the substance adsorbed to the particulates (per unit mass of particulates) over the dissolved concentration of the solute. The particulate adsorbed contaminant is represented as:

$$P = R_p M \qquad \text{(Eq. 2-3)}$$

where

P is the concentration of adsorbed contaminant (M/L^3), and

R_p is the mass of chemical per unit mass of particulate (M/M).

The partition coefficient may be represented as:

$$K_p = R_p/C \qquad \text{(Eq. 2-4)}$$

where

K_p is the partition coefficient (L^3/M).

This relationship assumes instantaneous partitioning between the dissolved and adsorbed forms of a contaminant. It is only valid for very low concentrations of the solute so that a linear approximation to the adsorption isotherm may be made.

2.3. HYDROLOGIC TRANSPORT PROCESSES

A wide variety of physical processes occur in natural water bodies which are important, to varying degrees, in the analysis of pollutant fate and transport. A more detailed description of these processes is given by Fischer et al. (1979) and Schnoor (1985). Some of the important hydrologic transport processes include:

Advection -- Transport of water flowing in a particular direction (more or less horizontal), such as water flowing due to the current in a stream or river.

Convection -- Vertical transport of water due to density gradients. This is a form of transport where the driving forces of the currents are density gradients resulting from temperature differences in deep lakes, and temperature and salinity differences in estuaries.

Molecular Diffusion -- Scattering of particles by random molecular motion, commonly characterized by Fick's law of diffusion.

Turbulent Diffusion -- Scattering of particles by random turbulent motion (advective transport via turbulent motion in the form of eddies).

Shear -- Mixing due to variations in the fluid velocity at different positions in the water body. One example of this could occur in a lake where a significant decrease in temperature occurs with depth, thereby causing a thermal resistance (resistance of colder and, therefore, denser and lower-lying water to be displaced by warmer, lighter and higher-lying water). A shear plane divides the surface currents that follow the wind from the return currents that run counter to the wind (Fair et al., 1968).

Dispersion -- The scattering of particles due to the combined effect of shear and diffusion (molecular and turbulent). Usually the combined effect of shear and transverse diffusion, represented as an effective dispersion, is orders of magnitude greater than other diffusive mechanisms acting in the direction of flow in rivers and estuaries.

Particle Settling -- The sinking of particles having densities greater than the fluid of the water body, such as sediments or suspended solids.

Particle Deposition -- The settling of particles from the water body to the underlying bed.

Particle Entrainment -- The picking up or lifting of particles from the underlying bed of a water body by turbulent motion over the bed.

In most water quality models, the processes of molecular and turbulent diffusion and shear are combined as a dispersion coefficient. This assumes that the mixing from all of these processes may be combined and represented by an equation similar to Fick's law of diffusion (i.e., the flux is proportional to the concentration gradient). The dispersion coefficient is the coefficient of proportionality used to relate the flux to the concentration gradient. In addition to these processes, estuary models that are formulated as tidally

averaged (averaged over a tidal cycle) also combine any intra-tidal advective transport into the dispersion coefficient. In contrast to true Fickian diffusion, where the diffusion coefficient is only a function of the diffusing material, the resulting dispersion coefficient is a specific characteristic of the water body, i.e., strongly dependent on the flow patterns, and must be determined in the calibration process or via experimental measurements on the specific water body of interest.

2.4. ATTENUATION MECHANISMS

The primary physical, biological, and chemical processes included in various water quality models are hydrolysis, oxidation-reduction, photolysis, ionization, volatilization, sorption, and biodegradation, and ionization. The kinetic formulation and rate constants used to describe these processes are based on laboratory measurements. The results of the laboratory measurements are incorporated in the water quality models as source or sink terms in the general advection-dispersion equation.

The transfer of controlled experimental results to natural aquatic systems is not always straightforward. Uncertainties arise in the definition of driving forces such as the available light for photolysis, sensitivity to temperature and pH of the natural system, availability of additional ions which may catalyze or retard various reactions, and atmospheric conditions. In spite of the uncertainties, these processes are incorporated in many water quality models, and some models have been calibrated to field conditions. Models that are carefully calibrated have been shown to be useful for representing the transport and transformation of various chemicals.

Most of the available models use some form of first-order reaction kinetics to represent the different processes that will degrade or transform a specific chemical. For a simple first-order reaction, ignoring all

other mechanisms, the concentration can be represented as a first-order differential equation:

$$\frac{dc}{dt} = -kc \qquad \text{(Eq. 2-5)}$$

where k is the rate constant (1/T). While in the simpler models the rate constant does not change, in the more complex models the rate constant(s) may be variable due to changing environmental conditions. The analytical solution to Equation 2-5 when k is a constant is:

$$C(t) = C_o\ e^{-kt} \qquad \text{(Eq. 2-6)}$$

where

$C(t)$ is the time-dependent concentration (M/L^3), and

C_o is the initial concentration (M/L^3).

From this equation an estimate of the time, t, required for the process to reduce the contaminant concentration below a fixed "action level" can be determined as follows:

$$t = \text{Ln}\ \{[C(t)/C_o]/(-k)\} \qquad \text{(Eq. 2-7)}$$

Often the reaction rates of various chemicals subject to different kinetic processes are characterized in terms of their half-life, $t_{1/2}$. This is a measure of the time required for some kinetic process to degrade or transform the specific chemical to one-half of the initial concentration. The half-life is calculated from Equation 2-7 with $C(t)/C_o$ set to 1/2.

A brief description of several important transformation processes is included for potential users unfamiliar with the terminology. Much more detailed descriptions including assumptions, limitations, kinetic formulations, and methods for estimating rate constants are given by Delos et al. (1984) and Neely and Blau (1985).

2.4.1. Hydrolysis

Hydrolysis is the breaking of bonds in a molecule due to reaction with water. Typically a compound is altered in a hydrolytic reaction by the replacement of some chemical group of the compound with a hydroxyl group. The hydrolysis reactions are commonly catalyzed by the presence of hydrogen or hydroxide ions, and hence the reaction rate is strongly dependent on the pH of the system. Hydrolytic reactions alter the structure of the reacting compound and may change its properties. Depending on the specific reaction, the new compound is usually less toxic than the original compound. Neely (1985) lists several functional groups that are susceptible to hydrolytic reactions, including alkyl halides, amides, carbamates, carboxylic acid esters, epoxides, lactones, phosphoric acid esters, and sulfonic acid esters. For many functional groups, and therefore a considerable number of compounds, hydrolysis will not occur.

2.4.2. Oxidation-Reduction

Oxidation-reduction reactions involve the transfer of electrons from the reduced species to the oxidized species. The oxidation-reduction potential is an important process in that it can control the oxidation number of the metals present in solution and may also change the oxidation state and structure of organics. Oxidation-reduction reactions are used in models in the form of mass action equations with resulting equilibrium constants related to stability. The primary difficulty in applying these reactions to environmental models is

that many redox reactions are very slow, and the concentrations of some species may be far from those predicted via thermodynamic equilibrium. In addition, some redox reactions are catalyzed by metal ions. Some compounds in which redox reactions have been observed to be important include mercury, toxaphene, and DDT (Tinsley, 1979).

2.4.3. Photolysis

Photolysis is the degradation process whereby radiant energy in the form of photons breaks the chemical bonds of a molecule. Direct photolysis involves direct absorption of photons by the molecule. Indirect photolysis involves the absorption of energy by a molecule from another molecule that has absorbed the photons. In indirect photolysis, the two steps are usually combined and the photochemical reaction is characterized by first-order kinetics. The reaction rate is dependent on the energy required to break the chemical bonds, available light intensity, and the presence of intermediate compounds making indirect photolysis possible. Characterization of light intensity as a function of depth, time of day, time of year, and dissolved particulate matter in the water column is difficult. These problems add uncertainty to the use of laboratory-derived photolysis rates in field conditions. Mill and Mabey (1985) describe the types of photolysis reactions affecting a variety of compounds including chloroaromatics, ketones, and aldehydes.

2.4.4. Volatilization

Volatilization is a physical transfer process where a chemical is transferred between the water body and the atmosphere at the water-air interface. For volatile materials, such as benzene, volatilization is an important process in understanding environmental fate in water. The two-film or two-resistance model of Whitman (1923) is a commonly used method for estimating a rate constant, and first-order kinetics are used to represent the transfer process.

Mass transfer rates are easily measured experimentally. Uncertainty in scaling the laboratory rates to natural systems is complicated by variations in velocity, depth, stratification, salinity, wind speed, and diurnal atmospheric conditions.

2.4.5. Sorption

Sorption is a transfer process whereby dissolved chemicals in the water become attached to sedimentary materials. The process is commonly described using a partition coefficient. The definition of the partition coefficient is the ratio at equilibrium of the amount of chemical sorbed on the solid phase divided by the amount of chemical left in solution, as shown in Equation 2-4. The important assumptions in using this formulation are: (1) the chemical is at trace concentrations, and hence the sorption isotherm may be assumed to be linear, and (2) the system is at equilibrium.

Some problems associated with field application of this concept include: (1) rapid movement of water and sediments in rivers and estuaries may not satisfy the assumption of system equilibrium; (2) some chemicals may exhibit nonreversible sorption characteristics; hence, desorption from sediments to the water column may not be correctly represented; (3) different particle sizes (sand, clay, and silts) exhibit different properties and should be accounted for separately; and (4) salinity in estuarine systems may affect the sorption process. Some of the compounds that may be strongly affected by sorption include heavy metals and many hydrophobic nonpolar compounds.

2.4.6. Biodegradation

Biological transformations are reactions due to the metabolic activity of aquatic microbes, primarily bacteria. Depending on the specific chemical, the transformations may be very fast due to the presence of enzymes; for other compounds the process may be very slow. For chemicals where the transformation is

fast, biodegradation is often the most important transformation process in the aquatic environment. Various kinetic formulations have been proposed, including first- and second-order forms. The rate coefficients are known to be a function of temperature, pH, and available nutrients. The second-order kinetic formulations describe the degradation rate as a function of the concentration of the compound and the size of the bacteria population, which is changing as the compound is degraded. A variety of organic compounds may be subject to biodegradation; a discussion is provided by Klecka (1985).

2.4.7. Ionization

The fate of toxic organics that are either acids or bases can be strongly affected by the concentration of hydrogen ions in a water body. To the same extent, organic chemicals that partition among the gaseous, solid, and solution compartments could be determined from acid-base interactions between chemical and the aqueous or soil/sediment components of the environment. Since many toxic organics seem to exist in very low concentrations and are at best only weak acids or weak bases, they will have little influence, if any, on the pH values of the water. The hydrogen ion concentration of the water will, however, determine whether acids or bases exist in neutral or ionic forms (Mills et al., 1985).

An organic acid or base that is extensively ionized could be markedly different from the corresponding neutral molecule in solubility, adsorption, biocentration, and toxic characteristics. For example, the ionized species of an organic acid is generally absorbed by sediments to a much lesser degree than is the neutral form. The solubility of an ionic form of an organic chemical will likely be greater than for the neutral species. Therefore, as a chemical is ionized under environmental conditions, the change in physical properties as well as the chemical reactivity will change with pH. The pH values found in

most aquatic systems range from approximately pH 4 to 9, with extreme values down to pH 2 and up to pH 11.

3. MODEL STRUCTURE

The choice of model structure is dependent on a variety of physical parameters related to the water body, the source terms, and the biochemical properties of the pollutant of interest. There are a variety of surface water models applicable to the types of water bodies the reader will need to analyze, which include streams, rivers, lakes, estuaries, and oceans. However, the methods by which these models are applied for each type of water body could be distinctly different. Water bodies, depending upon which type one is analyzing, may be dominated by different mixing and transport processes. For example, rivers are dominated by advective transport because water flow is in one direction and may move quite rapidly. For lakes, the dispersion process dominates because lake water is usually slow-moving, allowing the contaminant to spread and mix within the volume of water.

A simple example of the difference between a lake and a river is shown in Figure 3-1. The mixing and transport processes that control a lake usually require a model that can simulate concentration changes by depth. In this case, the lake has two vertical compartments representing the water column, and a third compartment representing the bed. Longitudinal compartments may not be necessary for a lake, since water movement out of the lake can be very slow. For a river, the mixing and transport processes are controlled by advection, and the model used requires concentration changes by distance downstream. Longitudinal compartments are more important, while understanding concentration changes by depth may not be as important.

This chapter describes the mixing and transport processes that are most important for each type of water body. In addition, some relatively simple equations are presented which may be used to provide an initial estimate

of dispersion coefficients and mixing distances appropriate for water bodies. The representations of dispersion coefficients and mixing distances are based on theoretical and empirical considerations, along with analytical solutions to Equation 2-1. The available models generally require a user-defined dispersion coefficient as an input parameter. This may be a single or spatially variable value, depending on model requirements. The equations given in this chapter are meant to provide an initial estimate for dispersion coefficients. The estimated values will most likely need to be refined in the calibration phase of a modeling study.

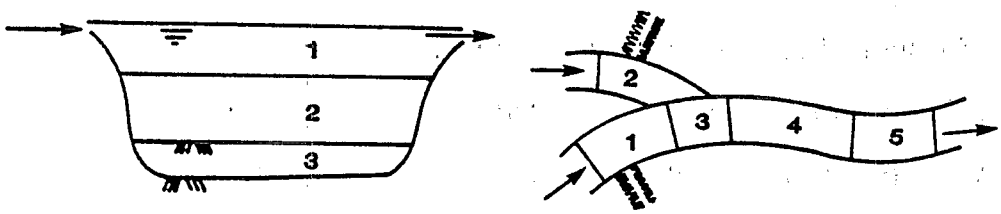

Figure 3-1. Vertical representation of a lake and longitudinal representation of a river.

3.1. RIVERS

The dominant transport process in most rivers is advection. Mixing over the vertical water column usually occurs rapidly as a result of shear flow and turbulent diffusion. An initial estimate of a vertical mixing coefficient is given by Fischer et al. (1979) as

$$E_V = 0.067\ du^* \qquad \text{(Eq. 3-1)}$$

where

E_v is the vertical mixing coefficient (L^2/T),

d is the depth (L), and

u^* is the shear velocity (L/T).

The shear velocity is defined as

$$u^* = \sqrt{gdS} \qquad \text{(Eq. 3-2)}$$

where

g is the acceleration of gravity (L/T^2), and

S is the channel slope (L/L).

Transverse mixing in natural rivers and channels is dependent on a wide variety of factors which may generate transverse motion within the stream. These factors include curves in the channel, groins, and variations in geometry. A useful estimate of the transverse mixing coefficient is given by Fischer et al. (1979) as

$$E_t = \alpha\, du^* \qquad \text{(Eq. 3-3)}$$

where

E_t is the transverse mixing coefficient (L^2/T), and

α is a coefficient that varies from approximately 0.4 to 0.8.

Using this transverse mixing coefficient, and assuming that vertical mixing is very rapid, estimates of the downstream distance for approximately uniform lateral mixing are given by Fischer et al. (1979) as

$$X = 0.1\ U\ W^2/E_t \quad \text{(for centerline discharge)} \qquad \text{(Eq. 3-4)}$$

and

$$X = 0.4\ U\ W^2/E_t \text{ (for side discharge)} \qquad \text{(Eq. 3-5)}$$

where

X is the distance downstream of the point source where the distribution across the stream is nearly uniform (L),

W is the stream width (L), and

U is the mean cross-sectional velocity (L/T).

These formulas are useful in the absence of field data for identifying the point at which a one-dimensional analysis is adequate. The uniform lateral mixing formulas are based on an analytical solution to the advection dispersion equation. The definition of approximately uniform lateral mixing used in these equations is that the concentration is within 5% of its mean value everywhere on the cross section. If a one-dimensional analysis is used in a situation where uniform lateral and vertical mixing has not occurred, the model results will be likely to underestimate the peak concentrations. In effect, the mass of contaminants will be spread uniformly over the cross-section rather than being limited to some smaller portion of the channel.

If a different definition of uniform lateral mixing is deemed appropriate for a specific application other than that stated above, Figure 3-2 may be used to estimate the numerical coefficients used in Equations 3-4 and 3-5. Figure 3-2 is based on an analytical solution to Equation 2-1 with a constant point source term at X = 0, a stream with a uniform depth and velocity, where the effects of dispersion in the longitudinal direction are considered minimal. The boundaries are represented by the superposition of image sources. The y axis represents the ratio of the concentration at the stream boundary, at a specific cross-section, to the peak concentration, and the x axis represents a dimensionless distance downstream.

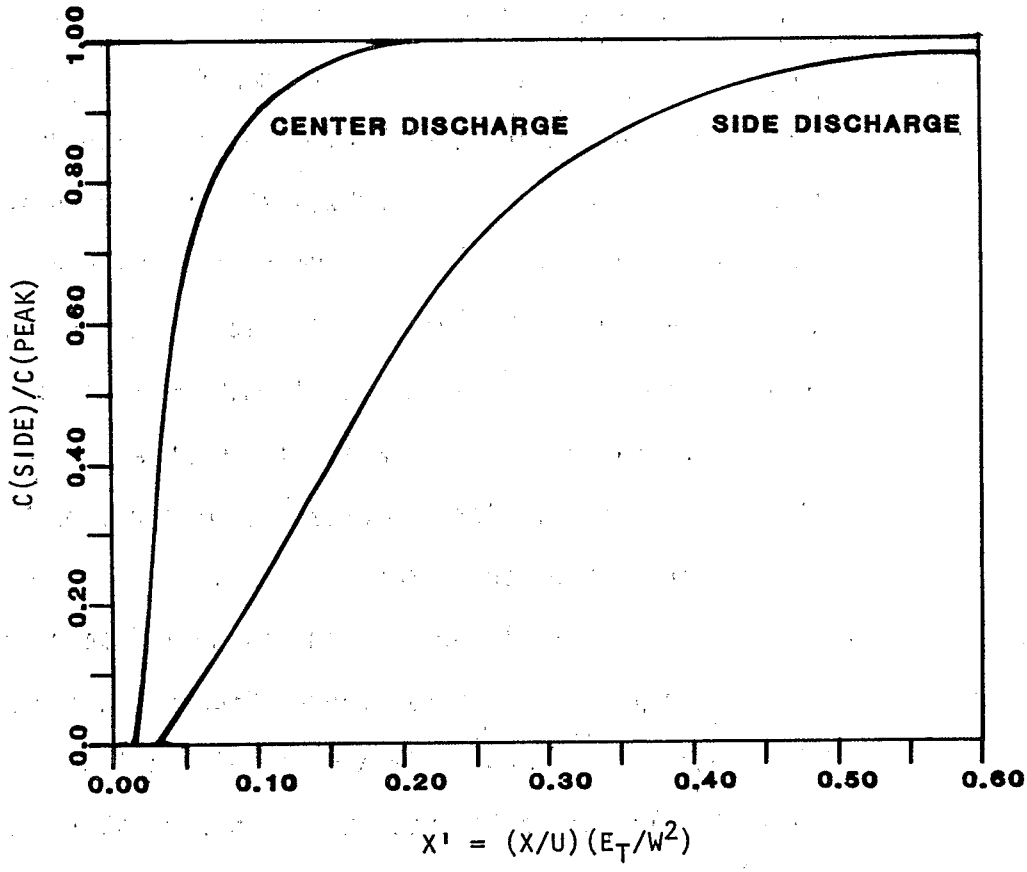

Figure 3-2. Ratio of boundary concentration to centerline concentration as a function of dimensionless downstream distance.

Probably the most difficult part of contaminant transport studies in rivers is related to the interactions with suspended and bed sediments. Various water quality models treat the sediment transport process with varying degrees of sophistication, and may be separated into three very broad classifications. The most sophisticated models in terms of sediment transport (SERATRA, CHNTRN, HSPF), examine the processes in a mechanistic fashion, describing scouring, settling, resuspension, and finite sources of bed sediments. The next level of models (WASTOX, TOXIWASP) requires that the user specify the sediment transport terms, including fluxes and dispersive terms, and the models calculate the resulting concentration of both suspended sediments and the sediment in the bed. The simpler models (EXAMS, SLSA, WQAM) require that the user specify the concentration of suspended sediments and any flux terms.

In all of these models, some of the terms describing the sediment transport processes must be treated as calibration parameters. The calibration parameters are adjusted to fit field data. For the most sophisticated models, the important parameters, such as erodibility coefficients, critical shear stress coefficients, and grain size distributions may sometimes be determined from laboratory experiments. However, it may often be necessary to treat some of these parameters as calibration coefficients. It should be stated that one estimate of a model parameter does not necessarily fix the validity of the model. However, the more information that is available and specific to a particular modeling analysis, the greater the understanding of the uncertainty associated with the computed results. If a situation arises in which a model is used and the available field data are limited, caution should be used in interpreting the model results, since under conditions of limited field data, the model results may be open to technical criticism even though the choice of the model was justified.

The incorporation of sediment contaminant interactions is important for situations where the contaminant of interest has a high affinity for adsorption. If the sediment contaminant interactions are not incorporated, the predicted concentration of dissolved contaminants in the water column would be higher than actually exists. If the contaminated bed sediments are ignored, the potential for a long-term source of pollution through resuspension and desorption cannot be fully evaluated.

3.2. LAKES AND RESERVOIRS

A variety of different transport mechanisms are active over different time frames in lakes and reservoirs. The one relatively constant transport mechanism is diffusion. This is because, even without mechanical mixing, the concentration of substance in solution will eventually become uniform (Fair et al., 1968). Other important mechanisms are advection due to wind stresses and convective transport as a result of surface cooling and the resulting unstable density structure. The time frame of advective mixing due to wind stresses is commonly short (hours to days), and complete mixing of the water body may not result. Convective overturn on an annual or biannual basis may completely mix the water body.

Historically, water quality models for lakes have basically followed two lines of development: (1) From an engineering point of view, model developers have tried to characterize circulation and exchange processes while simplifying the aquatic ecosystem; and (2) from the point of view of aquatic biology, model developers have tried to represent biological interactions and kinetics of different life stages, while simplifying transport processes and often representing the water body as a continuously stirred reactor (CSTR). The type of model appropriate for the exposure assessment of toxic chemicals must lie between these two extremes.

A common characteristic of many lakes and reservoirs is stratification on a seasonal basis. When a lake is stratified it is roughly separated into two layers: the upper layer of warmer water, referred to as the epilimnion; and the lower, more dense layer of colder water referred to as the hypolimnion. The boundary between the two layers is the thermocline, where a rapid change in temperature profile occurs. The vertical transport across the thermocline is often dominated by unpredictable events, such as wind-induced eddies, storm surges, and internal seiches. Generally these processes are not represented with a mechanistic formulation, but rather as diffusion processes.

An understanding of the reader's modeling objectives will help define the appropriate type of model structure in terms of necessary spatial dimensions and temporal characteristics. If the objective of the study is to identify the long-term accumulation of some conservative material over many years, the appropriate time step may be on the order of seasons or a year. The mixing processes within a reservoir over the time frame of a year may be relatively predominant; hence, a zero-dimensional single-compartment analysis may be the best choice of model structure. This type of analysis will provide a spatially averaged concentration that is appropriate for problems such as long-term accumulation.

In contrast, any analysis attempting to identify peak concentrations or the extent of a contaminant plume from some specific source will require the analysis of some spatial dimensions. The dimensionality of a model used for water quality in a lake will depend on several factors. If the lake is stratified, the vertical compartments will need to be analyzed. At a minimum, the vertical compartments of the lake should include the epilimnion and the hypolimnion. The necessity of analyzing longitudinal compartments will depend on the source terms and the degree of lateral mixing. Point source terms--for

example, a pipe discharge--may indicate that the lateral dimensions need to be evaluated, whereas nonpoint source terms--for example, soil runoff--may justify the use of a laterally averaged model.

The residence time of a lake is another important parameter in defining appropriate model structure. The residence time is defined as the theoretical length of time it take for a liquid to pass through the lake, assuming that all of the liquid moves through the lake at the same uniform velocity. Residence time can be determined by taking the volume of a lake and dividing by the incoming river inflow. For large deep lakes or reservoirs, the residence time may be on the order of several years and, in many cases (some exceptions exist), vertical one-dimensional models may be appropriate. This is because the lake's "flushing" time is very long and chemical reactions by depth are more likely to occur. For smaller reservoirs, such as run-of-river reservoirs, the residence time may be on the order of a week, and significant longitudinal concentration gradients may exist. In these cases, the longitudinal dimension should also be analyzed. When the "flushing" time of the lake is short (weeks), the type of chemical reaction that occurs by depth may not be as likely, and therefore one may wish to analyze only surface or near-surface problems.

Sediment contaminant interactions are important in lakes for any contaminant that has a high affinity for particulate matter. The actual sedimentation processes are usually much simpler than those encountered in rivers in that the primary process is the settling and deposition of particulates, with a smaller amount of resuspension due to diffusion and physical mixing at the bed. Over a long time period (on the order of 10 years), this interaction in deep lakes is important and must be evaluated.

3.3. ESTUARIES

Estuaries are probably the most complex water bodies in terms of hydro-

dynamic flow and the resultant mixing processes. In addition, formulating various physical, chemical, and biological transformation processes in estuaries is complicated by variations in salinity, both spatially and temporally. An estuary is defined as a semi-closed coastal body of water that is subject to tidal action and in which the sea water is measurably diluted by fresh water (Rich, 1973). In real time and three-dimensional space, the dominant transport mechanism is advection. However, water movement in an estuary varies significantly from that in a stream. In those reaches of a river that are subjected to tides, the motion of the water is caused not only by flow due to gravity but also by the rise and fall of tides, density currents (due to salt and freshwater movement), and wind effects. Toxic compounds released into such an estuary are mixed with water and are gradually diminished in concentration as they are transported back and forth over many tidal cycles. If a model is formulated to account for tidally averaged values, all of the advective transport due to tidal excursions is combined into one tidal mixing term, which is referred to as an effective dispersion coefficient.

Various classifications of estuary types have been suggested by different authors based on hydrodynamic conditions, geomorphological characteristics, time scales, and geometry. For the purposes of this report, the most useful classification is based on the following three major hydrodynamic or stratification categories, which were suggested by Pritchard (1967) and are shown in Figure 3-3:

(1) Sharply stratified estuaries, such as fjords and salt-wedge types, where the fresh water inflow flows over the top of the heavier salt water; examples include Puget Sound, Washington, and the Mississippi River estuary in Louisiana.

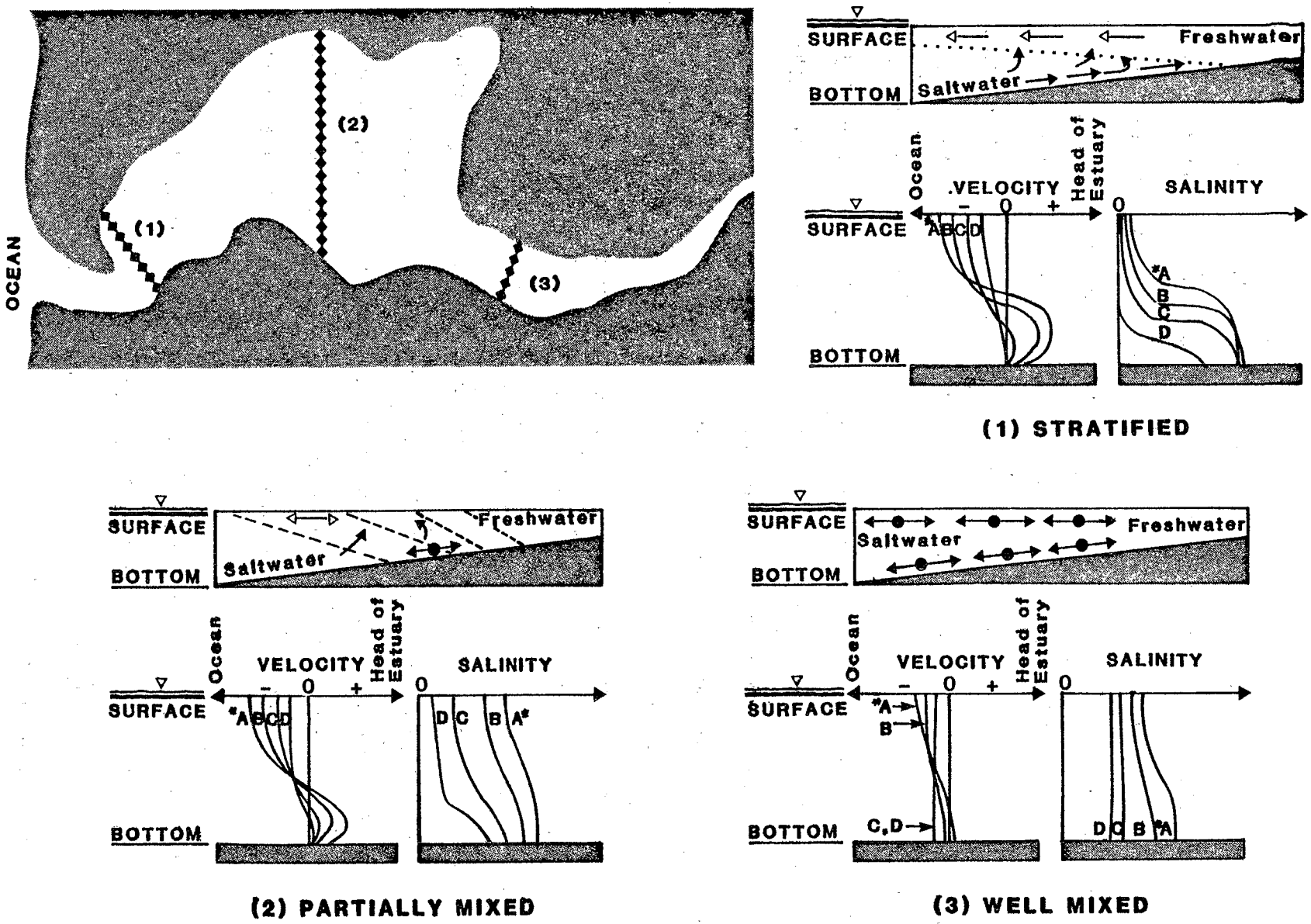

Figure 3-3. Classification of estuarine stratification.

SOURCE: Walton et al., 1984.

(2) Partially stratified estuaries where significant vertical density gradients exist; examples include the James River estuary, Virginia, and the Chesapeake Bay.

(3) Well-mixed estuaries where the salinity profile is nearly uniform over the vertical column; examples include San Francisco Bay, California, and San Diego Bay, California.

This type of classification is useful for defining the necessity of modeling the vertical dimension within the estuary. Complications with these categories often arise as a result of large storm events, which may change the stratification characteristics, and in cases where different portions of a given estuary fit different general classifications.

Other estuarine classifications are discussed in varying degrees of detail by Fischer et al. (1979), Walton et al. (1984), and Mills et al. (1985). Additionally, the last two references describe some of the characteristics of many estuaries in the United States, and list how specific estuaries fit the different classification schemes. In order to determine how a specific site fits the hydrodynamic or stratification categories, several simplified analysis techniques are available. The first is referred to as an "Estuarine Richardson Number" by Fischer et al. (1979), and is discussed in more detail in Chapter 4. The second means is the use of a stratification circulation diagram (Hansen and Rattray, 1966). This methodology is discussed by Fischer et al. (1979), Walton et al. (1984), and Mills et al. (1985), and the reader is referred to those sources. These simplified analysis techniques are useful tools. However, there is no substitute for direct field observations of the different characteristics of a water body.

Different estuaries may exhibit significant longitudinal and/or lateral variations, and site-specific analyses must include measurements in the study area to capture these variations. Some of the important parameters to measure include salinity, temperature, velocities, and dispersive characteristics.

The primary driving forces causing circulation are usually tidal wave action and fresh water inflows. Secondary forces are usually the wind stresses and internal density variations as a result of fresh water and salt water inflows. In some wide estuaries the Coriolis effect, due to the earth's rotation, may also affect circulation. For example, the Coriolis effect may cause a water flow to drift to one side as it moves down from a channel (Mills et al., 1985). The circulation within an estuary causes the advective transport of contaminants and several other dispersive mechanisms. The first dispersive mechanism is the result of shear and turbulent diffusion, as in rivers, except that flow direction and magnitude are continually changing. In stratified estuaries, this dispersive mechanism is complicated by the fact that the surface layer of less dense fresh water must exhibit a net tidally averaged seaward velocity. The lower layer of more dense salt water may, in contrast, exhibit a tidally averaged landward velocity. This phenomenon is referred to as a current reversal, where the tidally averaged currents in the stratified layers flow in opposite directions. If a contaminant is discharged in a region of an estuary where a current reversal exists, the contaminant plume may split into two clouds, with the cloud in the upper layer traveling seaward and the cloud in the lower layer traveling some distance landward. Obviously, a one-dimensional, longitudinal model cannot represent this phenomenon, and a longitudinal and vertical analysis, at a minimum, is necessary.

The second dispersive mechanism is referred to as "tidal pumping" or residual circulation. A detailed description of this mechanism is given by

Fischer et al. (1979). A simplistic description of the process is that the incoming flood tide may flow through some constriction forming a sort of jet, whereas the outgoing ebb tide flows from throughout the estuary towards the constriction. The end result is large circulation patterns or gyres on the landward side of the constriction.

The third dispersive mechanism is referred to as "tidal trapping" by Fischer et al. (1979). A brief description of tidal trapping is that different regions or zones of an estuary will have velocities less than that of the main channel due to greater frictional forces. In these regions the tidal wave will not propagate as far upstream. On the outgoing ebb tide, the particles or contaminants that have not traveled as far upstream will reach the main channel ahead of those that traveled farther upstream, and an effective mixing or dispersive mechanism will occur.

The estimation of empirical forms for vertical, transverse, and longitudinal mixing coefficients applicable to estuaries is a difficult process. For very wide estuaries with irregular cross-sections, no simple equations are available, and experimental measurements are the only suitable estimation techniques. For other estuaries that are relatively long, narrow, and uniform, similar to rivers, some empirical relationships are suggested by Fischer et al. (1979). These empirical relationships are of the same form as those suggested for rivers. The general form of the relationship for transverse mixing coefficients is the same as in Equation 3-3, but with different coefficients.

$$E_t = \alpha d u^* \qquad \text{(Eq. 3-6)}$$

where

E_t is the transverse mixing coefficient (L^2/T), and

α is a dimensionless empirical coefficient.

The results of several experiments by various scientists are described by Fischer et al. (1979) indicating that a very approximate range for the parameter α is between 0.4 and 1.6. The slope term, S, used in Eq. 3-2 is not defined in an estuary, an alternative estimate of the shear velocity, u^*, is

$$u^* = 0.1\ U \qquad \text{(Eq. 3-7)}$$

An approximate estimate of the vertical mixing coefficient is

$$E_V = 0.0024\ d\ V_A \qquad \text{(Eq. 3-8)}$$

where

E_V is the vertical mixing coefficient (L^2/T), and

V_A is the depth mean amplitude of the current (L/T).

This coefficient is suggested for uniformly mixed estuaries at mid-depth. Several other more complex relationships are suggested for stratified systems. The reader is referred to Fischer et al. (1979), pp. 249-251, for more details. In addition, a number of assumptions, limitations, and caveats for the simplified expressions are also described. It is advised that the reader consult this specific reference before using these equations to estimate mixing coefficients.

The sediment transport processes occurring in estuaries are similarly complex when compared to those occurring in rivers, and include scouring, resuspension, settling, and finite sources of bed sediments. In terms of sediment contaminant interactions, the processes are more complex due to the time scale and spatially-variable salinity occurring in estuaries. The salinity may affect various sorption processes along with other kinetic reactions. For this reason, the kinetic rate constants used in estuarine modeling should be spatial-

ly variable and, in some cases, temporally variable. If a single or constant coefficient is used, greater uncertainty is introduced into the modeling results.

3.4. TEMPORAL SCALE

The temporal variation used in a water quality model may be classified as dynamic (time-varying) or steady-state. Types of temporal variation are discussed in Thomann (1972) and are shown in Table 3-1. In a steady-state model, all variables are considered to be constant over time. The constant variables include source terms, flow rates, any boundary conditions, and the resulting spatial concentration distributions. In a transient model, some variables are considered to be changing in time. However, not all transient models consider all variables to be time-dependent. For example, some models may allow transient source terms under steady flow conditions. At the very least, they must consider source terms and resulting concentration distributions as time-variable. Additional categories are sometimes referred to as quasi-dynamic or quasi-steady-state. These terms are usually applied to models where a source term is assumed to be constant for a long period of time until steady-state concentrations are reached, at which point the source term is removed and the time required for the system to "cleanse" itself is calculated.

TABLE 3-1. FACTORS AFFECTING TEMPORAL SCALE

Waste load input	Water flow velocity, reaction coefficient	Water quality output
Constant	Constant	Constant
Time-variable	Constant	Time-variable
Constant	Time-variable	Time-variable
Time-variable	Time-variable	Time-variable

The basic difference between a transient model and a steady-state model is that the transient model has a "memory" of the initial state or previous condition of the system, which may correspond to a different source strength or flow rate. In a steady-state model, the previous or initial conditions do not affect the results. When applied to identical flow conditions and source terms (i.e., both constant) the steady-state model will predict a single spatially variable concentration distribution with a peak value. In contrast, a transient model starting from specified initial conditions will predict a series of time- and spatially variable concentration distributions that will initially have peak concentrations less than that predicted by the steady-state model. At some point in time, the transient results will asymptotically approach the steady-state results.

The time required for the transient results to approach steady-state conditions is highly dependent on the system being analyzed. For example, the water column at a specific point in a river has a very short "memory" of previous conditions due to the strong influence of advection, and will approach a steady-state condition relatively quickly. In contrast, the bed sediments in a river respond much more slowly to changes in source terms, and will only very slowly approach a steady-state condition. In reality, because of changes in flow rates and other factors, bed sediments may never actually reach a true steady-state condition.

In most applications in which a steady state model is used, the model may be applied to a variety of different conditions in a Monte Carlo* analysis. From this type of simulation a probability density function of the concentration

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*Monte Carlo refers to a statistical simulation which allows the prediction of the expected probability distribution of the model results based on the distribution of model inputs. This technique allows estimation of the predicted uncertainty of the model results.

may be developed which may be used to estimate the probability of exceeding some exposure level. A comparison between the frequency distributions developed from a steady-state and a transient model is described by Mulkey et al. (1982). The conclusions are applicable to concentrations in the water column in rivers where the loading terms are constant but the flow rate is variable. The conclusions cannot be generalized to bed sediments, lakes, or estuaries where different processes are important (i.e. dispersion, detention time). The frequency distribution derived from the Monte Carlo simulations with a steady-state model were nearly the same as the frequency distributions derived using a continuous-simulation model.

A variety of factors will influence the choice between a dynamic or a steady-state model. Important factors include source terms, hydrologic conditions, atmospheric conditions, biological effects, and attenuation processes. If the source terms in the water quality analysis are strongly time-varying, a transient analysis is necessary. Examples of time-varying source terms include accidental spills, seasonal application of pesticides and fertilizers, and, perhaps, intermittent discharges from industrial sources where some process is only performed on an occasional or irregular basis. Some steady (or nearly steady) source terms may include sewage treatment plant discharges and industrial wastes. Some source terms may have a daily variation that can, in some cases, be treated as a steady continuous source.

A hydrologic condition of importance when choosing between a steady-state and transient model is the flow rate. For lakes and rivers, if the flow rate is known to be relatively constant, the hydrologic conditions would indicate the use of a steady-state model. A common methodology is to use historic records of low flows and to assume that the lower volumes of water and longer residence times will give conservative estimates of concentration (overpredict).

The dynamic nature of flow in estuarine systems indicates that a transient analysis should be used. Steady-state analysis of highly variable systems such as estuaries should be used with extreme care, and only as a general screening tool. Hinwood and Wallis (1975) state that a steady-state model is inappropriate for short estuaries where the tidal excursion distance is a significant portion of the total length. Additionally, they state that a steady-state model will be unsatisfactory if the waste load, river inflow, or tidal range vary appreciably with a period close to the flushing time of the area of interest. An additional subclassification within the dynamic category is a tidally averaged analysis, which only applies to estuarine systems. A tidally averaged analysis will use a time step greater than a tidal cycle, while a more detailed dynamic description may use a time step on the order of 10 to 20 minutes. If a steady-state or tidally averaged model is used, extreme care must be taken to identify the effective dispersion coefficients used to represent all of the intra-tidal transport processes.

Variability in atmospheric conditions may also affect the choice between a dynamic or a steady-state model. The important atmospheric conditions include solar insolation, which affects heat transfer and resulting stratification, and degradation via photolysis; wind speed, direction, and duration, which affect volatilization and mixing of surface layers; and seasonal climatic changes, which affect heat transfer, stratification, and volatilization rates.

The time frame associated with studying biological effects should be available in the selected model. If a pollutant is acutely toxic and exposure for very short time frames must be examined, a model capable of analyzing short time frames is necessary. If a pollutant is only toxic when exposures occur for very long periods, this particular criterion may indicate the use of a steady-state model. The importance of different attenuation mechanisms must

also be considered along with the temporal characteristics of the model.

An important physical characteristic, unrelated to time variability, is the ratio of the volume of the estuary to the river inflow. In a steady-state analysis, the only advective transport is the result of river inflows. All of the tidally induced phenomena are represented by a dispersion coefficient. Walton et al. (1984) offer one example, as an extreme, of a closed-end canal system where there is little or no inflow and, hence, no advection towards the outlet. The analysis will depend entirely on the calibration of a dispersion coefficient. For any estuarine system where the freshwater inflows are small, this type of analysis is likely to be subject to large errors if applied to any conditions different than those used for calibration.

If a dynamic analysis (time-varying) is necessary, the selection of the proper time step (hours, days, months, or years) becomes very important. The factors influencing the choice of a time step will include stability criteria for numerical integration, and time variability of source terms and other driving functions. The stability criterion is a model-dependent parameter that should be described in a user's manual. Generally, the criterion is a relationship between the spatial resolution and the time step; the use of a coarser-grid resolution will usually enable the use of larger time steps at the expense of spatial accuracy. Limiting stability criteria may also arise from the rate constants associated with degradation processes; a simple example is provided by Walton et al. (1984). Explicit integration techniques commonly require smaller time steps for stable solutions than those required for implicit integration techniques, which are also subject to stability constraints for nonlinear problems. The time variability of source terms and other driving functions are problem-dependent parameters that must be identified by the user.

If a steady-state model is used in a problem where the source terms are time-variable, the steady-state results will probably underpredict the peak concentrations. The reason for this is that the transient nature of the source term will be averaged over the on and off periods; hence, the average source strength will be lower than the transient peaks. If a different source-term averaging procedure is used, such as a constant source at the peak transient rate of discharge, the model results may overpredict the peak concentrations. The use of this type of source-term averaging is likely to complicate the calibration process because the mass of contaminant input to the system will be too large. Attempting to match some observed concentrations with the model results will overestimate dispersive or degradation mechanisms.

3.5. DIMENSIONALITY

The choice of the number of spatial dimensions to be incorporated in a given analysis should depend primarily on whether or not a contaminant is completely or uniformly mixed over a given spatial dimension. The best means of resolving this issue is through field measurements of the contaminant of interest or some other conservative or nonconservative substance with known degradation rate, discharged at the same location.

For any estuary or reservoir, one should first determine whether or not the water body is stratified. If the water body is stratified, the vertical dimension should be analyzed. With a few exceptions, the analysis of large reservoirs with long residence times has traditionally been simplified to a one-dimensional vertical problem. This approach is probably adequate for contaminant problems resulting from nonpoint source terms. However, it should be used cautiously for problems with point source terms where mixing over horizontal directions may take a significant amount of time. If this type of analysis is used where uniform horizontal mixing has not occurred, the peak

concentrations in the vicinity of the source terms will be underpredicted by the model.

The flow patterns, mixing processes, and resulting transport in estuaries are very complex and are difficult to describe with one, two, or three-dimensional models. Specific situations where a one-dimensional (longitudinal) model may be appropriate include unstratified water bodies that are relatively long and relatively narrow. Three tests or criteria are suggested by Fischer et al. (1979) to determine the usefulness of a one-dimensional approach:

(1) The time scale for transverse mixing across the estuary is significantly less than the time required for the effluent to pass out of the estuary or for the substance to degrade. An estimate of the time scale for transverse mixing is given as $0.4W^2/E_t$, where W is the width of the estuary and E_t is the transverse mixing coefficient.

(2) The estuary is not significantly stratified, so that the contaminant may be assumed to be completely mixed over depth.

(3) Allowance is made in the analysis for higher concentrations near the source before cross-sectional mixing is complete.

As a final comment, the authors note that for practical reasons, a one-dimensional analysis is used in many cases even if criteria (1) and (2) are not met, but the results may be subject to larger errors.

For estuaries which are not relatively long, narrow, and uniform, the mechanisms of tidal pumping and tidal trapping may become important. These mechanisms are the result of variations in the geometry of the system, including both the bathymetry and constrictions. The complex geometry must, as a minimum, be represented using a two-dimensional (longitudinal, lateral) analysis. The vertically averaged models are only applicable to well-mixed (unstratified) estuaries, and currents are constrained to be entirely in the horizontal direc-

tions. Some estuaries which are stratified may be represented as a two-dimensional (longitudinal, vertical) system if the estuary is relatively long, narrow, and uniform. If the stratification is very distinct, as in salt-wedge estuaries, the vertical dimension may sometimes be represented by two layers. The final case is estuaries where stratification, tidal pumping, and tidal trapping are all important. Under these circumstances, a three-dimensional analysis may be necessary. Considerable expertise, along with extensive computational resources and funds, are necessary for the three-dimensional analysis of estuarine systems or any other water body.

For the analysis of contaminant transport in rivers, one-dimensional models are commonly used and are appropriate. The mixing length concepts presented by Fischer et al. (1979) and outlined earlier in this chapter are useful for determining where a one-dimensional analysis is appropriate. The limitation of a one-dimensional analysis in rivers would be to study the concentration levels near the discharge source or when the analysis involves a very wide river, on the order of 2,000 feet, where transverse mixing may not be complete for 10 to 100 miles downstream.

As a general rule of thumb for any water body, reducing the number of spatial dimensions analyzed may cause the model to underpredict the peak concentrations. If the water body is uniformly mixed over the particular spatial dimension, then dropping that dimension from the analysis is justified. If the contaminant is not uniformly mixed, such as near point sources, the model results should be interpreted with the full knowledge that peak concentrations will be underpredicted by the model.

3.6. DEGRADATION PROCESSES

A wide variety of degradation and transformation processes are known to affect the migration and fate of chemicals in the environment. Any process

that has been shown to affect a specific chemical should be incorporated into the analysis if possible. Most complex models incorporate the group of attenuation processes that were discussed in Chapter 2. Some models are formulated in such a manner that the user may easily specify additional processes as subroutines to the main program.

The determination of specific rate constants used in the kinetic formulations may be subject to substantial uncertainty. As a result, sensitivity studies must be performed to indicate which parameters contribute most to uncertainties. Through the use of sensitivity studies, some degree of confidence in the model results, or lack thereof, may be established. Additionally, the dominant processes may be identified and quantified better or formulated differently if possible.

If an important degradation process is not incorporated in the analysis, the predicted concentration of the affected chemical will be high. This problem may be complicated in the calibration process by the inappropriate adjustment of some other parameter, such as another rate constant or dispersion coefficient. This type of problem may have an important impact when the calibrated model is then applied to different conditions in a validation phase or a planning exercise. As a result, it is essential to incorporate all processes known to have a significant impact on the degradation of a particular chemical. It is also preferable to represent the processes individually rather than with a combined first-order decay term, so that the different environmental conditions affecting the different processes may be evaluated.

Another important problem that may arise if certain transformation processes are not incorporated is that some secondary or daughter substances will not be identified. If the secondary substances are not harmful, this is not a problem. If they are toxic, this is important because they may react differ-

ently (faster or slower, depending on the substances) than the original form of the chemical.

3.7. SEDIMENT TRANSPORT AND SORPTION PROCESSES

Many toxic substances are adsorbed onto particulates and may settle into bed sediments. As a result, the characteristics of the sediment transport process and resulting bed movement and accumulation are important factors in the identification of appropriate models. A useful classification structure is described by O'Connor and St. John (1982) and is included here. The three categories described are related to the mixing processes associated with the bed. The bed categories are: stationary, exchanging, and moving. These classifications are based primarily on the flow of water above the bed and the resulting turbulence and mixing processes. Another important mechanism is the role of sediment organisms in mixing the upper layer of sediments. This is most important in lakes where the other mixing processes are relatively small.

The stationary bed is characterized by very small or negligible horizontal motion. The primary water bodies where this condition is present would be very deep lakes and reservoirs that are not subject to strong mixing by winds. Under this rather idealized condition, the primary process is the accumulation of material on the bed. This process is described by a sedimentation velocity.

An exchanging bed is characterized by some amount of mixing in the upper layer of the bed, in addition to the sedimentation velocity. The mixing in the upper layer may be the result of biological action or shear resulting from fluid motion over the bed. The different types of water bodies where this condition may exist include rivers with low to moderate flows, lakes or regions within lakes where the wind effects extend to the bottom, and some estuaries or regions of estuaries where the velocities and tidal mixing effects are not dominant.

A moving bed is characterized by both mixing and advective transport of the bed sediments. The velocity over the bed is strong enough to cause erosion and resuspension of the sediments and to horizontally transport the suspended and bed materials. This type of bed condition may require a detailed or mechanistic description of the sediment transport process. The types of water bodies where this condition may be found include streams and rivers, under moderate to high flow rates; and estuaries or regions of estuaries where the velocities and tidal mixing effects are strong. Mechanistic descriptions of sediment transport have been studied for many years by hydraulic engineers primarily interested in the sedimentation of rivers and some reservoirs. These studies have concentrated primarily on coarse-grained materials, such as sands and gravel. In contrast, the sedimentary materials to which most contaminants are adsorbed are finer materials, such as clays and organic matter. Limited data are available regarding the characteristics of the finer-grained materials.

The models using a mechanistic description of sediment transport include SERATRA, CHNTRN, and HSPF for rivers, and FETRA for estuaries. The basic advantage of these models is that when calibrated and used in an analysis where a sediment transport characteristic is substantially different than calibration conditions, such as flow rate, results can be interpreted with more confidence. In most cases, the disadvantage of these mechanistic models is the lack of required input data (e.g., critical shear stress coefficients, erodibility coefficients, grain size distributions).

The sorption process whereby dissolved contaminants become adsorbed to particulates in the water column and bed sediments is represented in two different ways among the existing models. The majority of the models use a partition coefficient. The use of a partition coefficient assumes that the contaminant is at trace concentrations, so that the sorption isotherm is approx-

imately linear. Additionally, it assumes instantaneous equilbrium. A few models (SERATRA, FETRA, and HSPF) incorporate sorption as a first-order rate process which approaches an equilibrium condition defined by the partition coefficient.

The importance of incorporating sediment-contaminant interactions depends primarily on the sorptive characteristics of the pollutant of interest. The sorption process is a mechanism whereby a contaminant is removed from the water column. The relative importance of this mechanism is dependent on the partition coefficient of a particular contaminant and particulate concentration. If this process is not incorporated, the model results should overpredict the concentration of dissolved contaminants, and ignore the contaminant concentration in the bed sediments. For any transient problem, the contaminated bed sediments may also act as a relatively long-term contaminant source to the water column after the original source has ended.

3.8. NONPOINT SOURCE RUNOFF

Nonpoint sources of pollution, both from agricultural and urban areas, may constitute a significant portion of the pollutant loading rates to surface water bodies. The recognition of this problem is relatively new (the last 10 to 20 years), and, therefore, the analytical tools for evaluation of the problem are less developed and validated, relative to models developed for water bodies. The physical processes and spatial variability involved in surface runoff, sediment transport, and dissolved contaminant transport are very complex and are difficult to characterize from a fundamental, conservation-of-mass point of view. Accordingly, the available models all use varying degrees of empirical equations to represent the physical processes.

The physical processes are based on the hydrologic cycle. The important mechanisms incorporated, to varying degrees, in different runoff models include

precipitation, evapotranspiration, overland flow, and groundwater recharge/discharge. The various mechanisms important to the evapotranspiration process include: interception, depression storage, and transpiration by plants. Surface runoff or overland flow is the primary means for the transport of sediments and dissolved contaminants from the land surface to a water body. Groundwater discharge is another pathway for dissolved contaminants to reach the water body.

Within the overland flow, various sediment transport processes are important. They include bed load, contact load, saltation load, and suspended load. The primary kinetic process included in most runoff models is adsorption and desorption. Other processes may be present, but in many models it is assumed that the time scale of the runoff process, on the order of hours, allows one to ignore the other transformation processes until the pollutant has reached a water body. A few models also evaluate the transport of dissolved contaminants.

The available models for the analysis of nonpoint source pollutants can be generally placed in three categories, based on their purposes and formulations (Horner et al., 1986):

(1) Simple pollutant yield models,

(2) Empirical loading functions, and

(3) Nonpoint source simulation models.

Other categories are suggested by Huber and Heaney (1982) and Reckhow et al. (1985).

3.8.1. Simple Pollutant Yield Models

The pollutant yield models generally specify pollutant loading rates, due to runoff, as a function of the product of a concentration and a runoff rate.

The pollutant concentration must be measured or estimated from available literature. Some methods incorporate an exponential decay to the source term as a means of representing a first-flush effect after a deposition period.

The pollutant yield models are commonly applied to a design storm of selected frequency and magnitude. No routing of the pollutant from source areas to the water body is included, and no adsorption or desorption phenomena are explicitly analyzed. The methods are useful for a screening-level analysis, and are somewhat more suitable for urban areas with larger amounts of impervious area than for agricultural areas.

3.8.2. Empirical Loading Functions

The most common empirical loading function is the Universal Soil Loss Equation (USLE) by Wischmeier and Smith (1965). The original form of the equation was developed to predict erosion losses from croplands in the midwestern United States. The USLE is intended to generate mean annual results, not specific event results or annual results for a specific year. The form of the equation is:

$$Y(s) = R_f \cdot K_f \cdot L_f \cdot S_{gf} \cdot C_f \cdot P_f \qquad \text{(Eq. 3-9)}$$

where

$Y(s)$ is the sediment yield (mass/unit area-year),

R_f is the rainfall factor, expressing the erosion potential of average annual rainfall (product of the kinetic energy of rainfall, in units of length-mass/area, times average annual maximum 30-minute rainfall intensity of all significant storms, in units of depth/hour),

K_f is the soil erodibility factor (mass/unit area-unit R),

L_f is the slope length factor (dimensionless ratio),

S_{gf} is the slope gradient factor (dimensionless ratio),

C_f is the cover factor, accounting for land surface features (dimensionless ratio), and

P_f is the erosion control practice factor (dimensionless ratio).

This equation was developed to estimate sediment loss from an agricultural plot. Additional work by other researchers has resulted in modifications of this equation to account for sediment delivery from the plot to the water body (McElroy et al., 1976). A variety of modifications to the general form of the USLE have been utilized by various authors, and a review is included in Horner et al. (1986).

3.8.3. Nonpoint Source Simulation Models

Simulation models attempt to represent the major important processes of the hydrologic cycle. Generally, the hydrologic portion of these models is based on the conservation of mass (volume of water). The watershed is represented as one area or a series of subareas. Within specific areas, the watershed is separated into a group of storage zones. The transfer of water between the storage zones is represented by empirical transfer functions. The size of the storage zones and the coefficients of the transfer functions are problem-dependent parameters that need to be defined in the conceptualization and calibration phases of the modeling study.

One of the earliest nonpoint source simulation models was the Stanford Watershed Model (SWM) (Crawford and Linsley, 1962). The model simulates the runoff of water from a watershed. Many of the existing transport models use the framework of the Stanford Watershed Model as the basis of the hydrologic portion of modeling analysis.

The nonpoint source simulation models are the most complex class of runoff models. It is important to note that they still rely on some empirical rela-

tionships, as do the pollutant yield models and empirical loading functions, and hence, are quite sensitive to the calibration process. When properly calibrated, they have been shown to be capable of reproducing measured data. When calibrating the simulation models, two issues must be addressed. The first is based on the volume of runoff, and the second is based on the concentration of contaminants in the runoff. In general, these models are better able to reproduce the volume of runoff than the contaminant concentration in the runoff. This is due to a variety of factors, including the complexity of the different processes, the availability of reliable calibration data, and the dependence of concentration estimates on runoff volumes. Without sufficient field data to calibrate the model, the results may not be accurate.

The selection of a nonpoint source runoff model should depend upon the objective of the exposure analysis and the desired accuracy of the model results. For example, a simple objective would be to evaluate the effects of runoff into a lake on an annual basis. If the purpose is to identify the contaminant inputs into a specific water body, such as a lake, on an annual basis, the simplest choice is a modified form of the USLE. If the objective is to evaluate the effects of runoff on a time-varying scale, a continuous simulation model is a better choice. A continuous simulation model would provide much more detailed and somewhat more accurate time-dependent information, but at a much higher cost. The continuous simulation model should be able to give the user more accurate results by incorporating specific characteristics of the watershed and regional weather patterns. If all of the detailed time-dependent pollutant loading data are to be averaged into an annual loading rate, the justification for using a continuous simulation model is small, and the user should consider a model that incorporates annual time scales.

4. IDENTIFICATION OF MODEL PROCESSES

In order to select a model appropriate for a specific situation, the modeler must first identify those transport and degradation processes which are the most important or dominant factors. However, before a model is selected, the analyst should attempt to determine whether or not a potential contamination problem exists. If an existing site is being considered, this determination should be accomplished via direct field measurements. If the analysis is designed to evaluate the potential effects where an actual contaminant discharge has not occurred, a screening-level or preliminary exposure assessment analysis is necessary. Probably the best name for this step of the modeling study would be an order-of-magnitude analysis.

A variety of screening procedures for different types of water bodies are described by Mills et al. (1985). These screening procedures start from simple dilution calculations and proceed to slightly more complex analytical solutions, including some forms of transport and first-order degradation. These types of analysis can usually be performed with a hand calculator. In virtually every situation, the screening procedures of analysis should be performed before the process of model selection for a more detailed analysis is started.

The first level of a screening procedure, when evaluating potential contaminant concentrations in a water body, is to estimate the dilution based on the contaminant discharge divided by the river flow rate. This approach is called mass balance, and is shown in Equation 4-1.

$$C = \frac{\dot{m}}{Q} \qquad \text{(Eq. 4-1)}$$

where

C is the concentration in the river (M/L^3,)

$\dot{m}$ is the mass discharge rate to the river (M/T), and

Q is the flow rate of the river (L^3/T).

Mass balance makes the assumption that the mass of the contaminant is uniformly mixed across the water body. For exposure purposes, the assumption is that the receptor is exposed to the average concentration given by $\dot{m}/Q$. If uniform mixing occurs, this assumption is obviously true. Even if uniform mixing does not occur, the average or "expectation" value for the concentration may be the best number to use if the actual concentration to which the receptor is exposed is unknown. In the vicinity of the discharge, the mass balance approach may underestimate peak concentrations.

The next level of complexity in the screening procedure is to apply analytical solutions to the advection-dispersion equation in the vicinity of the discharge source. A variety of analytical solutions are available (Fischer et al., 1979; Mills et al., 1985). If the results of this screening procedure indicate that a predicted concentration is several orders of magnitude less than some regulatory standard or "safe" exposure level, then a more detailed analysis is probably not necessary. If the results of this approach indicate that a predicted concentration is within an order of magnitude, or greater than some regulatory standard or "safe" exposure level, then a more detailed modeling analysis may be necessary.

The value of the screening-level analysis is that it is simple to perform and may indicate that no significant contamination problem exists. It will also aid the user in conceptualization of the physical system, identification of important processes, and location and determination of available data. The assumptions used in the preliminary analysis should represent a reasonable worst-case condition (conservative), such that the predicted results over-

estimate potential conditions, limiting "false negatives."

If the field measurements and/or screening analysis indicate that a contamination problem exists, then a modeling study may be useful. The analyst must first identify the important processes to be incorporated in the modeling study. The remainder of this chapter describes some simple analytical means for comparing the importance of different processes that may be incorporated.

4.1. TRANSPORT PROCESSES

In order to assess the relative importance of different mixing, degradation, and transport processes, several techniques are suggested by Schnoor (1985), Eschenroeder (1983), and Fischer et al. (1979). The techniques include the use of dimensionless parameters and characteristic mixing times. Three characteristic mixing times are suggested by Eschenroeder (1983): advection time, t_A; diffusion time, t_D; and transformation time, t_T. The advection time is proportional to the principal length scale of the domain, l, divided by the mean velocity, u:

$$t_A \sim l/u \qquad \text{(Eq. 4-2)}$$

The diffusion time is proportional to the square of the transverse direction, W, divided by the dispersion coefficient, D:

$$t_D \sim W^2/2D \qquad \text{(Eq. 4-3)}$$

The transformation time is proportional to the reciprocal of the rate coefficient, k:

$$t_T \sim 1/k \qquad \text{(Eq. 4-4)}$$

These three parameters are very simple but quite useful in the model selection process. The basic concept is that if one specific characteristic mixing time is much smaller than the others, that process may transport or degrade the chemical before the other processes have a significant effect. If the transformation time is much smaller than the advection and diffusion time ($t_T << t_A$ and $t_T << t_D$) then there should be a rapid chemical change before significant movement occurs. In this case a far-field model may not be necessary because the chemical degrades in the near field. If the diffusion time is much smaller than the advection time and the transformation time ($t_D << t_A$ and $t_D << t_T$), then the process is dispersion-dominated, and contaminant may be spread nearly uniformly throughout the water body. In this case a box model, potentially a zero-dimensional (CSTR) analysis, may be appropriate. The last example described by Eschenroeder (1983) is the situation in which all three mixing times are of the same order of magnitude ($t_A \sim t_D \sim t_T$). In this situation, all three processes act simultaneously, and an appropriate model should include advection, dispersion, and chemical reactions.

The use of appropriate dimensionless parameters in the screening phase of an analysis is suggested by Fischer et al. (1979) and Schnoor (1985). The basic idea behind dimensional analysis is to define useful dimensionless groups of variables that describe physical and chemical processes and may provide the basis for comparisons between models and prototypes. Many dimensionless parameters have been derived, and it is not necessary for a modeler to rederive them. Rather, the existing parameters may be used as a means of estimating the importance of different processes.

The first dimensionless parameter to examine is the Peclet number, defined as

$$P_E = ul/D \qquad \text{(Eq. 4-5)}$$

where

u is the mean velocity (L/T),

l is the segment length (L), and

D is a dispersion coefficient (L^2/T).

This dimensionless parameter is a ratio of the advective transport process to the dispersive transport process. If the Peclet number is significantly greater than 1.0, the system is advection-dominated; if it is much less than 1.0, dispersion dominates the transport of dissolved conservative substances.

Another useful dimensionless parameter is referred to as a Reaction number, defined as

$$R_{XN} = kD/u^2 \qquad \text{(Eq. 4-6)}$$

where k is a first-order reaction rate constant representing a transformation process or combination of processes (1/T). This dimensionless parameter is the ratio of the combined effect of reactions and dispersion to that of advection. Schnoor (1985) suggests that if the Reaction number is greater than 10, the system may be approximated as completely mixed (under steady conditions). If the Reaction number is less than 0.1, advection dominates and a plug flow model (advection only, no dispersion) may be adequate. If the Reaction number is greater than 0.1 and less than 10, the analyst must consider both advection and dispersion as important processes. This same dimensionless parameter is referred to as an estuarine number by references cited in Southerland et al. (1984).

A third dimensionless parameter useful in identifying important processes in estuarine systems is called an "Estuarine Richardson Number" by Fischer (1972), and is defined as

$$R = [(\Delta\rho/\rho) g\ Q_f]/W\ U_t^3 \qquad \text{(Eq. 4-7)}$$

where

R is the Estuarine Richardson Number,

$\Delta\rho$ is the difference in density between the river and ocean water (M/L^3),

ρ is the density of the ocean water (M/L^3),

g is the acceleration of gravity (L/T^2),

Q_f is the freshwater inflow (L^3/T),

W is the channel width (L), and

U_t is the root mean square tidal velocity (L/T).

This parameter is a ratio of the input of buoyancy from the river, to the mixing power available from the tide. Estuaries with very large R may be expected to be strongly stratified, and those with very small R values are likely to be well mixed. A very approximate range suggested by Fischer et al. (1979) is that the transition from a well-mixed to a strongly stratified estuary occurs for ($0.08 < R < 0.8$).

4.2. DEGRADATION PROCESSES

The choice of important or necessary degradation processes to be incorporated into a model depends primarily on the chemical and physical properties of the contaminant of interest. Secondary in the choice of degradation processes are various properties of the water body which may have some effect on the transformation process. A simple example is related to the adsorption of a contaminant by particulate matter. If a contaminant has a high affinity for

adsorption, as do many hydrophobic compounds, the adsorption process will be an important part of the analysis. For compounds that have a relatively low affinity for adsorption, the process may not be as important; however, the characteristics of the water body need to be considered. If the sediment load in the water body is low, then ignoring adsorption should not have a significant impact on the results unless benthic concentrations are important. If the sediment load in the water body is very high, a significant amount of the contaminant may be removed from the water column even though the contaminant has a low affinity for adsorption.

In order to estimate the relative importance of the different degradation processes influencing the fate of pollutants in the aquatic environment, the reader is referred to several useful references: Callahan et al. (1979), Tinsley (1979), and Mills et al. (1985). Another good reference for estimating the importance of various degradation processes, along with methods for estimating specific rate coefficients, is Neely and Blau (1985). If some degradation or transformation process is identified as being important for a particular contaminant, then rate constants used in the description of the kinetic process must be estimated from a review of available literature or experimental measurements.

When examining different processes affecting a particular chemical, the half-life or some other representative decay time is a good indicator of which processes to incorporate and which to ignore. For example, if the different processes we wish to examine have time scales that differ by orders of magnitude (minutes versus days), then it is usually appropriate to focus on the process that has the much shorter decay time.

5. MODEL SELECTION CRITERIA

The purpose of this section is (1) to describe a specific series of steps, the selection criteria, that may be used in the process of evaluating the important physical and chemical characteristics of the study area, and (2) to match those characteristics with the capabilities of available models when used in exposure assessments. In the first part of this chapter, we discuss the formulation and structure of the selection criteria. In the second part, we discuss the specific selection criteria and how they apply to different types of water bodies. The final section includes a summary of some of the available models.

The selection of models for the analysis of exposure to contaminants involves factors addressing a number of issues, not all of which are amenable to expression in specific criteria. Certain judgmental factors are better suited to statement in the form of general guidelines and principles. Many of these guidelines and principles arise from the nature of the overall modeling process, of which model selection is but a single step. Five general steps may be identified in the modeling process. Although model selection is meant to be the primary emphasis of this report, the different steps influence each other and need to be described. The five general steps are:

(1) Problem Characterization -- The analyst clearly identifies the exposure assessment study objectives and constraints.

(2) Site Characterization -- The analyst reviews available data on the site, develops a conceptual model identifying processes of interest, and performs a preliminary exposure assessment. If a model study is necessary, the next step is to identify and obtain necessary data. The results of the site characterization will determine technical

specifications for model selection by identifying the significant processes at the site.

(3) Model Selection Criteria -- The analyst matches the objective, technical, and implementation criteria to available models and selects the most appropriate model(s).

(4) Code Installation -- If the model selected is a computer code, the code is installed on the computer system and tested to document proper installation and ability to reproduce accepted solutions to standard problems.

(5) Model Application -- The verified model uses site characterization data as input for the exposure assessment simulation.

These five general steps are not the model selection criteria, but rather the overall process by which a problem is identified and a model selected to perform an exposure assessment study. Model Selection Criteria is listed as the third step in this process. The two previous steps, Problem Characterization and Site Characterization, are crucial in the selection of appropriate model(s). While the steps can be considered sequential in nature, it is important to recognize interactions and feedback mechanisms between them. For instance, knowledge of the Model Selection Criteria is important to assure that Site Characterization is adequate and properly formatted. An understanding of Code Installation procedures is required for proper scheduling and resource allocation. Familiarity of candidate models is needed to assure that Site Characterization provides necessary input data.

The first step of the process, Problem Characterization, is important because a wide variety of models and modeling approaches are available. Different modeling techniques are suitable for different objectives and physical problems. The exposure assessment objectives must define what the goals of the

analysis should be and also must be defined in a manner consistent with known project constraints, such as schedule, budget, and other resources.

The second step of the process, Site Characterization, is an important step because the conceptualization of the physical system, whether it is a specific site or a generic problem, will obviously influence any additional steps. If the objectives of the exposure assessment are to evaluate an existing known contamination problem, then this step should include field measurements and/or review of available data pertinent to the specific study area. Depending on the specific type of water body, the field measurements may include: pollutant concentration, depth and channel characteristics, flow rate, velocity profiles, salinity profiles, temperature profiles, sediment characteristics, and overall dispersive characteristics. Field measurements may identify the extent of the contamination problem and whether or not the concentration levels are above some regulatory or dangerous level. In addition, if these initial studies identify a contamination problem and a modeling study is to be performed, then the field measurements will be used in the selection of appropriate model(s) and for model calibration.

If the objectives of the analysis are to evaluate a potential problem where an actual contaminant discharge has not occurred, then field measurements of pollutant concentration are obviously not possible. Under these circumstances a screening level or preliminary exposure assessment approach is necessary. The simplest screening analysis is described in Chapter 4. The results of a preliminary exposure assessment should indicate whether or not a more detailed analysis is necessary.

The third step in the process, Model Selection Criteria (the primary goal of this report), is entirely dependent on the first two steps. This step is covered in more detail in the rest of this chapter.

The fourth step, Code Installation, only applies when the model chosen in the third step is a computer code. When a code is first obtained and installed on a specific computer system, it is essential that the model be tested to verify that it is working correctly and can reproduce suitable example problems. Various computer systems and the necessary model software may have a variety of differences, some distinct and others more subtle. These differences may require some modification to an acquired code (e.g., changing output formats) on different computer systems. Verification assures that modifications have not changed model results significantly. This step should be performed by the individual doing the model analysis.

The fifth step of the process, Model Application, relates to the use of a model in an attempt to answer the questions defined in the objectives. Depending on the objectives of the analysis, this step may consist of several parts, including calibration, validation, and application of a model for different conditions or scenarios.

5.1. STRUCTURE OF THE MODEL SELECTION CRITERIA

The proper selection of a model is essential to the successful simulation of an exposure assessment for surface water systems. This section defines in detail Step 3 of the general modeling process, Model Selection Criteria.

The structure of the Model Selection Criteria is as follows:

(1) Objectives criteria specify the nature and intent of the analysis to be performed.

(2) Technical criteria specify the site-specific processes to be simulated by the model.

(3) Implementation criteria specify the quality assurance (QA) and documentation requirements.

The objectives criteria may be roughly classified as preliminary exposure assessment or site-specific (detailed) exposure assessment analysis. The study context and objectives determine the amount of uncertainty permitted, which in turn, together with the system characteristics, determine the degree of technical complexity required in the modeling process. The simplest exposure assessment models require restrictive assumptions regarding the dimensionality and time variability of the system, along with the formulation of kinetic processes. The more complex exposure assessment models may relax some of the restrictive assumptions; however, more extensive input data are usually required. The selection of simplified exposure assessment techniques can only be justified if the project objectives are defined as a preliminary exposure assessment and/or the technical specifications for model selection are satisfied (see next section). Implicit in the objectives criteria must be a realization of the available resources, including staff and money. When available resources are a limiting factor, the objectives of the study must be defined within the appropriate context.

The technical criteria for model selection are based primarily on: (1) physical mixing and transport processes; (2) biological, chemical, and physical degradation and transformation processes; and (3) geometry and/or dimensionality and time variability of the system. In Chapter 3 of this report, the important processes relative to different water bodies are described. In Chapter 4, simplified means are presented for assessing the relative importance of the different processes.

The implementation criteria are related to the degree of quality assurance (QA) and documentation to which a model has been subjected. It is preferable to obtain exposure assessment codes from federal agencies and departments where stringent QA procedures are in effect. Whenever possible, public domain codes

should be selected.

Documentation requirements refer to selecting models for which user's manuals and test verification documentation exist. Test problems for comparison should be available in the user's manual or from the source where the model was obtained. This requirement is necessary for step 4 of the general modeling process, Code Installation. It is not mandatory that such documentation exist for the selected model; however, it is strongly recommended that the analyst select standard, well-documented models, particularly if the model selected is a computer code. If possible, models should be selected for which site-specific simulations are documented in the open literature and for which the model results were compared with field data.

Other general aspects of Model Selection Criteria which should never override the objective, technical, or implementation criteria include schedule, budget, and staff and equipment resources. Time and cost constraints, as imposed by mandatory schedules and budgets, must be incorporated into the definition of project objectives and may dictate both the type of model selected and the general modeling approach. In cases where both the simpler and more complex models meet the selection criteria, one should then consider time to run the modeling analysis and projects costs as deciding factors. Time requirements will be important if staff are not familiar with any of the appropriate models. These constraints may require the use of a different modeling team that is experienced with the selected models.

Staff resources are also a major consideration in modeling. Regardless of the quality of the model selected, the expertise of the analyst has a major impact on model results. Staffing can also affect model selection when the analyst is familiar with one or more of the appropriate models. In the simplest case, if the analyst has direct experience with an acceptable model, then

that model is preferred. Similarly, if the analyst has experience with a particular type of model (e.g., finite element versus finite difference), one of that type should be selected. In certain cases, familiarity with a model more complex than required may dictate the use of that model, since there will be no loss of resolution and the added staff experience would compensate for time and cost differences. In no case, however, should familiarity with a model dictate its selection when it does not satisfy the objective, technical, and implementation criteria.

Hardware requirements and availability are also major considerations in modeling. The more complex mathematical codes require more powerful computers with larger mass storage devices and extra peripheral equipment. If both analytical models and those based on computer codes meet the selection criteria, available hardware may dictate the use of the simpler analytical model. If a sophisticated code is required and adequate equipment is not available, alternate means of conducting the modeling must be found. Equipment constraints should not be used to justify the use of a model that does not meet the selection criteria.

5.2. MODEL SELECTION PROCESS

This section describes the model selection process in detail. It is assumed at this point that a preliminary exposure assessment has been performed and the results indicate that a more detailed analysis is necessary. It is also assumed that data from the study area and contaminants of interest have been sampled and collected. Table 5-1 illustrates the selection process in the form of an outline. The remainder of this section describes in more detail important considerations related to each step of the outline. Wherever possible, we have provided some guidance with regard to potential errors (under-predicted versus over-predicted concentration levels) that may result from an inappropriate model choice.

TABLE 5-1. OUTLINE OF THE MODEL SELECTION PROCESS

I. INITIAL ANALYSIS

A. Identify project objectives
B. Identify contaminant sources
C. Identify chemical and physical properties of the contaminant

II. SELECTION OF A NONPOINT SOURCE RUNOFF MODEL

A. Identify the type and use of the land area
B. What time characteristics are necessary?
C. What are the spatial characteristics of the area?
D. Identify the important physical, chemical, and biological processes
E. Select a nonpoint source runoff model

III. SURFACE WATER FLOW

A. Identify the water body as a river, lake, or estuary
B. Is the water body stratified or well mixed?
C. Steady-state or transient analysis necessary?
D. One-, two-, or three-dimensional analysis?
E. Select appropriate model for surface water flow

IV. SURFACE WATER CONTAMINANT TRANSPORT

A. Point or nonpoint sources?
B. Steady-state or transient analysis necessary?
C. One-, two-, or three-dimensional analysis necessary?
D. What are the dominant mixing and transport processes?
E. Are sediment contaminant interactions important?
F. What biological, chemical, and physical reactions need to be incorporated?
G. Select appropriate model for surface water contaminant transport analysis

I. INITIAL ANALYSIS

I.A. Identify Project Objectives

The first step in the selection of a model or models is a clear definition of the purpose of the modeling study. What is the particular contaminant(s) of interest? Exposure assessment models are commonly used as predictive tools for the evaluation of chemical hazards and various pollution control scenarios. In defining the study objectives, some characterization of the acceptable uncertainty is necessary. The objectives and associated acceptable uncertainty must be defined in the context of the available budget, time and staff constraints. If available resources pose a limiting constraint, the study objectives may necessarily be defined as a preliminary exposure assessment analysis.

The types of methods or models used will depend upon the project objectives. For example, a three-dimensional, transient analysis may be required to identify maximum point concentrations resulting from a hypothetical spill of toxic materials. In contrast, a one-dimensional, or possibly a zero-dimensional, steady-state model may be appropriate for the analysis of nonpoint discharges into a lake. If an analysis is being performed to determine if a water quality standard is exceeded, the specific constraints of the standard may define several aspects of the appropriate model. Walton et al. (1984) refer to these constraints as regulatory scales. Examples of these constraints are allowable mixing zones near discharges and short time frames where some standard may be temporarily exceeded. A model that can resolve these characteristics spatially and temporally must be chosen.

I.B. Identify Contaminant Sources

The sources of the contaminants entering the water body need to be identified. The different types of sources may include instantaneous point sources due to spills, continuous point sources such as discharge from a pipe, and non-

point sources due to surface runoff. Along with the location and type of the contaminant sources, the specific contaminants of interest must be identified.

The identification of contaminant sources is a very important step that will help define the sequence of choices related to model dimensionality, time frame, and degradation processes. However, not all models may incorporate the types of source terms existing in the physical system. The obvious examples are point sources, such as a pipe discharge, versus distributed nonpoint sources, such as surface runoff, and transient source terms, such as a cyclic discharge or a spill, versus a continuous discharge.

I.C. Identify the Chemical and Physical Properties of the Contaminant

Once the specific contaminant of interest has been defined, the next step is to identify the chemical and physical properties of the contaminant. Many toxic chemicals are subject to a variety of degradation and transformation processes. Depending upon the chemical, only specific processes may be important. These processes may include hydrolysis, oxidation and reduction, photolysis, volatilization, ionization, and degradation due to biological activity. Another important process, sorption to sedimentary materials, may affect the fate of heavy metals and many hydrophobic compounds. To determine the chemical and physical properties of the contaminant may involve laboratory experiments and/or a review of the available literature. Sources of data available in the literature include Callahan et al. (1979), Mills et al. (1985), and Neely and Blau (1985).

II. SELECTION OF A NONPOINT SOURCE RUNOFF MODEL

Several approaches for the selection of specific pollutant runoff models are described by Reckhow et al. (1985) and Huber and Heaney (1982). The approach outlined in this section is from Huber and Heaney (1982).

II.A. Identify the Type and Use of Land Area

Land areas may be roughly classified as urban or nonurban, with a variety of subclassifications within each general category. Urban areas may be further subclassifie as residential, commercial, industrial, and open-space. The nonurban areas can be classified as agriculture, silviculture, and mining. Within the agricultural subclassification, important categories may include irrigated versus nonirrigated, different crop types, and tilled fields versus range land.

II.B. What Time Characteristics are Necessary?

The choice of particular time-dependent properties of different pollutant runoff models should depend on the modeling objectives. Three categories of time-dependence are incorporated in available models: (1) seasonal or annual average; (2) continuous simulation; and (3) single-event simulation. The continuous-simulation models use a time step on the order of 15 minutes to 1 day, and can be used to simulate study area conditions over one season or for several years. The single-event simulation models use a time step on the order of a minute, and are used to estimate runoff from a single rainstorm.

For a preliminary exposure assessment analysis, a long-term accumulation such as a seasonal or annual average model is probably the best choice. If project objectives include identifying peak time-dependent concentrations, a continuous-simulation model will be necessary. If a very detailed analysis of runoff is required, Huber and Heaney (1982) suggest that all three types of models be used in sequence 1, 2, 3. The annual average analysis is used as an initial approach, the continuous-simulation model is used to evaluate the dynamic nature of different and multiple storm events, and the single-event simulation is used to evaluate specific storm events determined to be the most crucial.

II.C. What are the Spatial Characteristics of the Area?

The physical size of the study area and whether multiple catchments or zones need to be defined in the model are important spatial characteristics of an area. The catchment size is important in determining whether or not flow routing is necessary. A "very crude rule of thumb" offered by Huber and Heaney (1982) is that routing effects should be considered whenever the catchment size is greater than 50 acres.

If the area of interest contains separate catchments with distinctly different land use practices, such as an agricultural area versus a forest, a model capable of simulating multiple catchments is necessary. Some models are designed to evaluate one specific area, such as an agricultural field, while others have multiple catchment capabilities.

II.D. Identify the Important Physical, Chemical, and Biological Processes

A significant physical characteristic is catchment size. In small catchments, flow routing may not be as important when compared to larger catchments. Snowmelt runoff is another physical process that affects nonpoint source runoff conditions. A physical process to consider in urban areas is runoff storage in engineered facilities. The interactions and degradation of different chemicals in the soil system and root zone may also be very important processes for determining the proper model for specific applications in agricultural areas. Models that treat these interactions are available, and may be the best choices to satisfy certain project objectives.

II.E. Select Nonpoint Source Runoff Model

After completing steps I.A, B, C, and II.A, B, C, D of the Model Selection Process, the user should proceed to Table 5-2, which is the summary matrix of nonpoint source runoff models. Using Table 5-2, the user should compare the capabilities and characteristics of the available models with the needs of the

TABLE 5-2. SUMMARY MATRIX OF NONPOINT SOURCE RUNOFF MODELS

Capabilities and characteristics	Model name									
	USLE	MRI	HSPF	NPS	ARM-II	AGRUN	ACTMO	CREAMS	SWMM	STORM
Applicable land areas										
Urban			X	X					X	X
Agricultural	X	X	X	X	X	X	X	X	X	X
Forest	X	X	X	X	X					
Spatial properties										
Single catchment	X	X		X	X		X	X		
Small	X	X		X	X		X	X		
Large										
Multiple catchments			X			X			X	X
Temporal properties										
Annual/seasonal	X	X								
Single event			X	X	X	X	X	X	X	X
Continuous simulation			X	X	X	X	X	X	X	X
Hydrologic processes										
Surface runoff			X	X	X	X	X	X	X	X
Subsurface processes			X	X	X	X		X		
Snowmelt			X	X	X		X		X	X
Flow routing			X			X		X	X	X
Storage			X					X	X	X
Water quality processes										
Sediment-erosion	X	X	X	X	X	X	X	X	X	X
Adsorption		X	X		X		X	X		
Conventional pollutants		X	X			X		X	X	X
Pesticides		X	X		X		X	X		
Conservative substances		X	X		X		X		X	
Nonconservative substances		X	X		X		X			

specific study, and select a model, or group of models, that best satisfies those needs.

III. SURFACE WATER FLOW

In the analysis of many water quality problems, the dominant mechanism for the transport of contaminants is the advection of dissolved and particulate contaminants by the flowing water. For this reason, it is necessary to characterize the flow patterns within the water body. Characterizing the flow within a water body could result in choosing one of several different strategies. These include extensive field measurements, limited measurements coupled with a numerical hydrodynamic model, and examination of historical records of flow rates. The rest of this section will deal with the selection of numerical hydrodynamic models. Under some conditions, such as a preliminary exposure assessment using a simple steady-state model, this surface water flow section can be bypassed if the user assumes only low-flow conditions.

III.A. Identify Water Body as a River, Lake, or Estuary

To choose a hydrodynamic flow model, one must first classify the water body as a stream or river, lake or reservoir, or estuary. Although these classifications seem fairly distinct, some cases may arise in which the classification is not clear and engineering judgment must be exercised. An example of such a classification problem could be the difference between a run-of-river reservoir and some upstream reaches of river estuary systems. Within these general categories, there are several subclassifications. Estuaries may be classified as well-mixed, partially mixed, or salt-wedge types. Lakes may be classified as shallow run-of-river impoundments with relatively short residence times (weeks), or as very deep impoundments with long residence times (years).

The proper classification of a water body will help determine the dominant transport and mixing process. In addition, the water body classification could

also help determine the correct choice of model dimensionality. Well-mixed estuaries may, in some cases, be adequately represented using a one-dimensional, longitudinal model. In contrast, a salt wedge or sharply stratified estuary will require, at a minimum, a two-dimensional, longitudinal, and vertical model to adequately represent the important transport and mixing processes. For the intermediate, partially mixed estuary, the selection of the model and the model dimensionality may not be obvious and will require additional judgment by the user. The model selection should depend on various factors, but should stay within the project objectives of the study (e.g., necessary accuracy).

III.B. Is the Water Body Stratified or Well Mixed?

The next step is to identify whether the water body is stratified or well-mixed over the vertical water column. This step does not usually apply to rivers. Stratification results from density variations due to temperature differences in lakes, and salinity and temperature differences in estuaries. Stratification is commonly a seasonal phenomenon in many lakes and in deep, fjord-type estuaries such as the Puget Sound. If stratification is significant within a particular water body, it is necessary to analyze the vertical dimension along with other spatial dimensions.

The best way to determine whether or not stratification exists is by examining measurements of salinity and/or temperature over the vertical water column. Approaches for estimating the density of water as a function of temperature and salinity are included in Fischer et al. (1979). If such measurements cannot be made or are not available, predictions of the degree of thermal stratification should be made as specified by Mills et al. (1985) for reservoirs. The same authors state that stratification may be the single most important phenomenon influencing water quality in many impoundments. The

Estuarine Richardson Number described in Chapter 4 can be used for determining the stratification for estuaries.

III.C. Steady-State or Transient Analysis

Once the water body is classified, the next step is to determine whether a steady-state or transient analysis is necessary. Several factors must be considered in this decision, including project objectives, contaminant sources, chemical and physical properties of the contaminants, and characteristics of the water body. A steady-state analysis would be appropriate for problems where the project objective is to identify waste load allocation procedures, the source terms are known or assumed to be constant, and the flow field is based on some minimum flow rate in a river. For any problems dealing with instantaneous sources, such as spills, a transient contaminant transport analysis is required, but a steady-flow analysis may be adequate if the flow field does not change significantly over the time frame of the analysis. Rivers and lakes could have flow fields that do not change significantly over the time requirements of the analysis.

For estuaries the flow system is dynamic, with approximately a twice-daily cycle. For contamination problems that occur at a single time (instantaneous sources), a dynamic flow field is necessary in order to understand the effect of the contaminants as they are carried away from the source. For contamination problems that occur over a long time period (continuous sources), a tidally averaged flow field could be appropriate. If a tidally averaged flow field is used, the model will require field measurements of salinity to determine the dispersion coefficients. The salinity measurements will help to characterize the intra-tidal advective transport that is not represented in the tidally-averaged analysis.

Where a transient analysis is used, two factors are important in defining the time step. The first factor relates to the time scale determined by project objectives, regulatory standards, and the rate of biological and chemical degradation. The second factor relates to stability criteria resulting from the implicit or explicit integration of the time-derivative terms in the governing equation. Individual models will have different stability criteria. The documentation and user's manual identify the time step and spatial resolution relationship necessary for stability.

III.D. Is a One-, Two-, or Three-Dimensional Analysis Necessary?

The dimensionality of the flow field analysis is also dependent on various factors including project objectives, source terms, and characteristics of the water body. When studying water quality problems due to nonpoint sources in lakes or rivers, a one-dimensional or, in some cases, for lakes, a zero-dimensional analysis (for example, a continuously stirred reactor) is adequate because of the uncertainty in measuring the actual nonpoint source. Almost all other water quality problems are initially three-dimensional in nature. Mixing processes, however, may distribute a contaminant uniformly or nearly uniformly over one or more spatial dimensions. In rivers, one-dimensional, longitudinal analysis is usually appropriate because mixing over the vertical water column occurs relatively quickly due to dispersion as a result of shear flow. Mixing in the lateral directions may also occur quickly. Situations where one-dimensional analysis in rivers is not appropriate are: (1) determining the contaminant problem near the actual point sources because vertical and lateral mixing may not be complete, and (2) when analyzing water quality problems in very wide rivers (2,000 feet wide) because lateral mixing may take 10 to 100 miles before it is completed. Analytical means for estimating the distance of uniform lateral mixing are described in Chapter 3. These methods are only approximate

and should be interpreted as such.

The use of one-dimensional, longitudinal analysis in well-mixed estuaries may be justified subject to the constraints discussed in Chapter 3. Other estuarine systems will generally require a two- or three-dimensional analysis, depending on project objectives. The existing two- and three-dimensional estuarine hydrodynamic models are quite complex and expensive to use in terms of both manpower requirements and computer costs. For the more complex models, considerable experience is necessary in order to apply and calibrate these models properly.

In most analyses of lakes with large residence times, a one-dimensional vertical analysis is used. This type of analysis necessarily ignores the horizontal circulation patterns resulting from wind stresses. Two- and three-dimensional circulation models for lakes exist, but they are more in the nature of research tools than the models considered herein. For run-of-river reservoirs with short residence times, on the order of weeks to months, the longitudinal variation of water quality may need to be examined in addition to the vertical water column.

III.E. Select Appropriate Model for Surface Water Flow

Incorporating all of the information in Sections I.A, B, C and III.A, B, and C, the next step is to choose a flow model with the necessary capabilities. Table 5-3 lists the capabilities of various flow models. The choice of models should be based on the listed criteria; if more than one model satisfies all the criteria, the simplest model should be chosen. A somewhat more complex model may be chosen based on availability and user familiarity. Another important factor in the choice may be that a particular contaminant transport model was developed to be used with a specific flow model such as CHNTRN (Yeh, 1982a) and CHNHYD (Yeh, 1982b). When a situation arises in which two particular

TABLE 5-3. SUMMARY MATRIX OF SURFACE WATER FLOW MODELS

Characteristics	Model name											
	HEC-2	CHNHYD	HEC-6	SEDONE	HSPF	DWOPER	DYNHYD3	EXPLORE-I	CAFE	WATFLO	Leender-tse-2D	Leender-tse-3D
Applicable water bodies												
River	X	X	X	X	X	X	X	X	X	X	X	X
Lake												
Estuary		X		X			X	X	X	X	X	X
Dimensions												
1-dimensional	1L	1L	1L	1L	1L	1L	1L	1L				
2-dimensional							Q2	Q2	2H	2H	2H	
3-dimensional												X
Time dependence												
Steady-state	X											
Transient		X	X	X	X	X	X	X	X	X	X	X
Solution technique												
Numerical	FD	FD	FD	FD	FD	FD	FD	FD	FE	FD	FD	FD
Availability												
Public domain	X	X	X	X	X	X	X	X	X		X	X
Proprietary										X		
Support												
Unknown		X		X				X	X		X	X
HEC	X		X									
U.S. EPA					X		X					
NOAA						X						
Contractual										X		
Other												
Sedimentation			X	X	X							
Water quality capabilities					X		X				X	
Compatibility with specific transport model							X	X	X	X		
Autocalibration						X						

LEGEND: 1L = one-dimensional longitudinal; Q2 = quasi-two-dimensional, link-node, horizontal plane; 2H = two-dimensional, horizontal plane; FD = finite difference; FE = finite element.

models are coupled together and they satisfy all the criteria, the logical choice would be a flow model because incorporating the results of a flow into a transport model is the least time-consuming procedure.

IV. SURFACE WATER CONTAMINANT TRANSPORT

After the flow field has been defined via field measurements and/or numerical models, the next step is to choose a water quality model to evaluate the transport and degradation of contaminants. A variety of available models are applicable to most water bodies where the flow field has previously been defined, including lakes, rivers, and estuaries.

IV.A. Point or Nonpoint Sources?

It is important to evaluate whether the model incorporates the types of sources necessary. If the model does not incorporate point and/or nonpoint sources, it may not be useful for the particular analysis. In some cases, nonpoint sources may be simulated as a series of point sources located along the boundary of the water body where the nonpoint runoff enters the system. This method should be adequate as long as the point sources mix together relatively quickly in relation to the length scale of interest.

IV.B. Steady-State or Transient Analysis?

The choice between a steady-state and a transient model is dependent on project objectives, source terms, and characteristics of the water body. Project objectives, such as waste load allocation and design of effluent standards, may allow for the use of a steady-state model. When project objectives are defined as a preliminary exposure assessment, where limited calibration data are available, a steady-state analysis may be the best approach.

Transient models may be necessary when the effects take place within short time frames and the concentration is rapidly varying. Steady-state models may be appropriate when the source terms are known to be steady in time, and also

in some cases where the cyclic variation in the source strength may be averaged over time.

The characteristics of a water body that pertain to the choice of a steady-state or a transient model include the following: For rivers, the flow rate and corresponding sediment transport; for lakes, the inflow/outflow rates and residence time; and for estuaries, tidal excursion distances, flushing time, tidal range, and river inflow rate. If the flow rate of a river is highly variable during the time frame of interest, a transient analysis is necessary. Very high flow rates will also significantly change the sediment transport characteristics that must be analyzed. For large and/or deep lakes with long residence times, a steady-state or annual analysis may be indicated by the flow conditions. For smaller lakes, a transient analysis may be necessary to account for variability in inflow and outflow rates and the corresponding residence times. In estuaries, if the tidal excursion distances are a significant portion of the total length, a transient analysis is necessary. If the tidal range or the river inflow rate varies significantly, a transient analysis is necessary.

If a steady-state model is used in a problem where the source terms are time-variable, the steady state results will underpredict the peak concentrations if the variable source term is averaged over time. If a different source term is used, such as a constant source at the peak transient rate of discharge, then the model results may overpredict the peak concentrations.

IV.C. <u>One-, Two-, or Three-Dimensional Analysis?</u>

The choice of dimensionality for the analysis of contaminant transport is similar to the choice of dimensionality for the flow model. The choice of the number of spatial dimensions to be incorporated in a given analysis should depend primarily on whether or not the contaminant is completely or uniformly

mixed over a given spatial dimension. If field measurements are available, the user should review the data to determine the contaminant mixing. If field measurements are not available, the user should review Chapter 3 (Equations 3-4 and 3-5) to best determine the choice of dimensionality.

For any estuary or reservoir that is stratified, the vertical dimension and the horizontal dimension should be analyzed. The analysis of large reservoirs with long residence times has traditionally been simplified to a one-dimensional vertical problem. For rivers, one-dimensional analysis is usually appropriate, except near point sources and for very wide rivers. The use of one-dimensional, longitudinal analysis in well mixed estuaries is justified subject to certain constraints described in Chapter 3. Other estuarine systems will generally require a two- or three-dimensional analysis, depending on project objectives.

In general, reducing the number of spatial dimensions analyzed may cause the model to underpredict peak concentrations. If a water body is uniformly mixed over a particular spatial dimension, dropping that dimension from the analysis is justified. If a contaminant is not uniformly mixed, such as occurs near point sources, the model results will underpredict the peak concentrations in that vicinity.

IV.D. <u>What are the Dominant Mixing and Transport Processes?</u>

The significant mixing and transport processes within the water body must be identified. These may include advection, convection, dispersion, molecular diffusion, turbulent diffusion, shear, mixing by plumes and buoyant jets, particle settling, and entrainment. The mixing and transport processes that are predominant depends upon the water body the user is analyzing. Several approximate means for determining the relative importance of different mixing and transport processes are described in Chapter 4.

As a general rule, advection in the longitudinal direction is necessary for analysis of rivers, while in some cases (steady-state analysis, high velocities) longitudinal dispersion may be ignored without significantly affecting results. In the analysis of estuaries, both advective and dispersive transport must be considered. In some seasonally stratified systems, convective transport due to unstable stratification must also be considered. In lakes with long residence times, dispersive and vertical convective transport are often the most significant processes. In lakes with short residence times, advective longitudinal transport is the most significant process.

IV.E. Are Sediment Contaminant Interactions Important?

Interactions between dissolved contaminants and particles should be examined for contaminants with high affinity for particulate matter. Another significant criterion is whether or not the water body has a significant sediment load. The different types of sediment may also be very important because experiments have shown that some contaminants may have a high affinity to adsorb to clays or organic material, and may have a lower affinity to adsorb to other, more coarsely-grained sediments.

The degree of complexity used in the analysis of sediment transport and contaminant interactions with the sediment depends upon the objectives of the analysis, the availability of data, and the type of water body under consideration. In the analysis of lakes and reservoirs, the sediment transport processes are much simpler than those occurring in rivers and estuaries, and the use of models in which the user specifies sediment fluxes is adequate. In rivers and estuaries under high flow rates, a mechanistic sediment transport model may be necessary to define sediment fluxes if the original objectives include any sort of extrapolation beyond existing or measured conditions.

IV.F. What Biological, Chemical and Physical Interactions Need to be Incorporated?

The final criterion for the selection of a water quality transport model is to identify the important biological, chemical, and physical interactions between the aquatic environment and the particular contaminant. Some models have been formulated such that other specific kinetic reactions may be easily incorporated by a user as subroutines. Other important characteristics of the contaminant include the degradation of original compounds into new compounds or into daughters of the original contaminant. Several technical documents are available which characterize the importance of different kinetic processes affecting a variety of chemicals. These include Callahan et al. (1979), Mills et al. (1985), and Neely and Blau (1985).

The majority of the water quality models addressed in this document incorporate all of the above physical and biochemical degradation processes. However, among the transport models there are some differences in the formulation of reaction kinetics. Just two of the twelve models, EXAMS and HSPF, incorporate reactions of the daughters of the primary compound within the original simulation. Some of the other ten models may be used to evaluate the degradation of the secondary substances using the results of previous model runs on the primary compound.

IV.G. Select Appropriate Model for Contaminant Transport Analysis

Using all of the previous information, the next step is to select a transport model. Combining the problem-specific information pertinent to each selection criterion with the model capabilities listed in Table 5-4, the user should select a model or group of models appropriate for the specific problem. The simplest model satisfying all of the previous criteria should be chosen. Somewhat more complex models may be used based on availability and user famili-

TABLE 5-4. SUMMARY MATRIX OF SURFACE WATER CONTAMINANT TRANSPORT MODELS

Characteristics and processes	Model name											
	WQAM	SLSA	MICHRIV	CATP	EXAMS	MEXAMS	WASTOX	TOXIWASP	CHNTRN	HSPF	FETRA	SERATRA
Applicable water bodies												
River	X	X	X	X	X	X	X	X	X	X	X	X
Lake	X	X		X	X	X	X	X		X		
Estuary	X						X	X	X		X	
Dimensions												
1-dimensional	B	B	X	C	C	C	C	C	X	X		
2-dimensional				C	C	C	C	C			2H	2V
3-dimensional				C	C	C	C	C				
Time dependence												
Steady-state	X	X	X	X	X	X						
Transient							X	X	X	X	X	X
Solution technique												
Analytical	X	X	X									
Numerical				FD	FD	FD	FD	FD	FD	FD	FE	FE
Sedimentation												
Settling	X	X	X	X		X	X	X	X	X	X	X
Exchanging bed		X	X		X	X	X	X	X	X	X	X
Transport							X	X	X	X	X	X
Scour/deposition							X	X	X	X	X	X
Degradation/transformation												
First-order decay	X	X	X	X	X		X	X	X	X	X	X
Photolysis					X		X	X	X	X		X
Hydrolysis					X		X	X	X	X		X
Oxidation					X		X	X	X	X		X
Biodegradation					X		X	X	X	X		X
Volatilization					X		X	X	X	X		X
Sorption	X	X	X	X	X	X	X	X	X	X	X	X
Daughter products					X					X	X	
Availability												
Public domain	X		X		X	X	X	X	X	X	X	X
Proprietary		X		X								
Support												
Unknown		X		X			X		X		X	X
U.S. EPA	X		X		X	X		X		X		

LEGEND: B = box model, one-dimensional for rivers, zero-dimensional for lakes; C = compartment model; 2H = two-dimensional, horizontal plane; 2V = two-dimensional vertical plane; FD = finite difference; FE = finite element.

arity.

5.3. DIFFERENT APPLICATIONS

The selection criteria are written primarily from the point of view of an analyst performing an exposure assessment study. The basic process begins with defining project objectives, assessing a physical situation, and then selecting a model to represent the important processes relevant to the project objectives and physical conditions. Another use of the selection criteria is from the point of view of a regulatory agency that is reviewing an exposure assessment study. Under these circumstances, the reviewer needs to evaluate the choice of the model used in performing the study. The selection criteria must be fundamentally the same for both applications; one to select a model, the other to determine if the model used is appropriate. This section is included to describe the differences in both applications.

The first step in reviewing the exposure assessment study is to identify the characteristics and capabilities of the specific model. Examples of model characteristics and capabilities are listed in the tables in section 5.4. The models shown in section 5.4 do not represent all available models; other models exist that may be appropriate for specific applications. A users's manual and description of the model is necessary in order to review the choice of a specific model (see implementation criteria, section 5.1). From a user's manual, the data relative to the different categories listed in Tables 5-2, 5-3, and 5-4 must be identified.

The single most important step in choosing a model is to define project objectives. Similarly for reviewing a model selection, the most important step must be to identify what the objectives of the study are. The objectives of the analysis should clearly state whether it is performed as a preliminary exposure assessment, or if a more detailed site-specific analysis, with appro-

priate data for calibration and validation, is intended. In cases where the objectives are not clearly defined, the only option is to interpret how the results and conclusions of the study are presented (e.g., associated uncertainty, potential impacts, and importance of decisions based on the results). This could be difficult and may require a subjective decision. After this initial step, the rest of the selection criteria are essentially the same for both the selection of a model and review of a model selection by another person.

It is important that the reviewer examine the presentation of results and conclusions to see whether they are consistent with the study objectives, model choice, and model application. A preliminary exposure assessment should incorporate uncertainty in the nature of an order of magnitude at least. For more detailed site-specific analysis, the validation phase of a modeling study may provide some guidance in defining the uncertainty associated with the model predictions.

A simple example illustrating the relationship between the project objectives, model choice, and results is as follows: Consider a preliminary exposure assessment of some hydrophobic compound where sorption is important. For a preliminary analysis, it is probably adequate to include all attenuation mechanisms, including sorption, as a combined first-order decay term, and some form of an analytical solution may be an appropriate model choice. The results should be presented as a screening-level (orders of magnitude estimate) of concentrations in the water column. This type of estimate is consistent with the project objectives and model choice. The analysis may not examine the accumulation of contaminants in the bed sediments (depending on the specific analytical solution) and, hence, no conclusions in relation to the importance of the bed sediments can be made. Another modeling approach must be used to evaluate

the accumulation of contaminants in the beds.

5.4. MODEL SUMMARY TABLES

Tables 5-2, 5-3, and 5-4 describe the capabilities and characteristics of a variety of different models that may be used in an exposure assessment study. The models included in the summary tables do not constitute an all-inclusive list of every available model. The user can choose from a number of other models that are available from a variety of sources. All of the models included in Tables 5-2, 5-3, and 5-4 have some form of documentation and/or user's manual. The properties of the models included in the tables were obtained by reviewing user's manuals, literature sources describing specific model applications, and literature sources reviewing available models.

The tables are to be used by first proceeding through the appropriate part of the selection criteria and noting the problem-specific characteristics relative to each selection criterion. This information will describe the needs of the specific analysis. The problem-specific needs may then be compared with the capabilities of available models and a model, or group of models, may be chosen which best satisfy the needs of the specific problem.

Table 5-2 lists the capabilities of nonpoint source runoff models. Table 5-3 lists the capabilities of surface water flow models. Table 5-4 lists the capabilities of surface water contaminant transport models. In terms of the degradation and transformation processes associated with the transport models, all of the models have a first-order decay term as a minimum. The first-order decay coefficient may be defined to incorporate all of the different attenuation processes. A single combined first-order decay coefficient will not allow the user to understand the variability of process as a function of changing environmental conditions. The models that incorporate a single combined first-order decay term are: WQAM, SLSA, MICHRIV, CTAP, and FETRA.

6. USE OF THE SELECTION CRITERIA

The purpose of this chapter is to show, by means of examples, how the selection criteria may be used. Two examples are included. The first relates to a preliminary exposure assessement, and the second is a site-specific evaluation of a complex real problem. The same physical problem is used in both examples, with different objectives defined for the two cases. The two examples are intended to illustrate that different project objectives will have a distinct impact on the modeling process and selection of appropriate models. As this document is used and applied to actual exposure assessment studies, future updates of this document will incorporate these studies.

6.1. DESCRIPTION OF EXPOSURE ANALYSIS PROBLEM

An exposure assessment group has been requested to perform an exposure assessment on a former chemical recycling plant in the western end of the State of Kentucky. Land disposal of solvents at the facility resulted in the contamination of the soils with heavy metals and organic and inorganic chemicals. The site is about 20 acres in size, and is bounded by a stream that leads to a larger river, which is used for drinking water supplies and aquaculture. Vegetation on the site consists of tall weeds, trees, and shrubs on approximately 2/3 of the site, with the remaining 1/3 barren due to roads, parking lots, and disposal areas.

A variety of contaminants have been measured in the adjoining creek, including benzene, toluene, trichloroethylene, and phenol. Samples of tissue from fish in the adjoining creek and further downstream in the river have indicated bioaccumulation of heavy metals. Much cleanup work has been performed at the site, and it is suggested that further work be done. The additional work will cost several millions of dollars, and the parties responsible for the

site question the amount of cleanup that is necessary. The decision will be based in part on the expected risk to the public and on potential impacts to the aquaculture facilities downstream.

The two levels of analysis, preliminary exposure assessment and detailed site-specific assessment, have substantially different data requirements. The preliminary exposure assessment will be based on a limited amount of field data. The field data may include: an estimate of the mass of contaminants disposed of at the site, a limited number of soil and surface water samples, an estimated low-flow condition for a stream or river, and estimates of the biochemical properties of the contaminants. The more detailed site-specific analysis will require additional data on the amount of surface runoff, the contaminant and sediment concentration in the runoff, precipitation and flow rate records, stream sediment transport characteristics and contaminant concentration in the stream sediments, and downstream samples of contaminant concentrations. As the study progresses, additional data may be necessary.

6.2. PRELIMINARY EXPOSURE ASSESSMENT

6.2.1. Initial Analysis

The objectives of the analysis are to provide a reasonable order of magnitude estimate of the concentration of contaminants in the water column. The first approach can be a relatively simple hand calculation. Using an estimated loading term from some modified form of the USLE, and a recorded or assumed low-flow condition, a simple dilution calculation could be generated. The uncertainty in this calculation could be large, with as much as several orders of magnitude difference from the actual contaminant concentration found in the water.

The preliminary analysis consists of two components. The first is to determine if a more detailed analysis is necessary. The second is to provide

estimated ranges in terms of flow rates and downstream distances at which sampling may provide useful calibration data. The primary concerns are the potential contamination of drinking water supplies and the bioaccumulation of the chemical in fish.

The constraints of the analysis are that it must be performed in a short time frame, with limited resources, and that little field data are available. With the limited amount of field data, the analysis is necessarily reduced to a preliminary exposure assessment. The only source of the specific chemicals entering the stream is from the land area surrounding the closed recycling plant. The specific contaminants to be analyzed are heavy metals, such as chromium, lead, mercury; and organics, such as trichloroethylene, phenol, benzene, and toluene. Based on data presented in Callahan et al. (1979), the following processes are important for the constituents of interest: sorption, volatilization, hydrolysis, and biodegradation. These processes should be incorporated into the model that is selected.

6.2.2. Selection of a Nonpoint Source Runoff Model

The land area is identified as an urban area that is relatively open and is adjoined by commercial and residential areas. Based on the defined project objectives of a preliminary exposure assessment and the limited field data with which to calibrate the model, an annual time scale is appropriate. The spatial characteristics of the area are that it is 20 acres in size and bounded on one side by a stream. It is assumed that the dominant mechanism for transporting the contaminants from the land area to the stream is particulate sorbed erosion. Based on this information, the project objectives, and the assumptions, the MRI nonpoint source loading functions would likely be the best approach. The project objective of a preliminary analysis, in terms of required accuracy and lack of calibration data, are the primary factors involved in this choice.

The timing of the nonpoint source loading, which the MRI analysis cannot provide, will be important, and the assumptions regarding streamflow rates and loading terms must be made in a conservative manner. If a more detailed analysis is necessary after the preliminary exposure assessment, further data will be collected and a more complex model will be selected.

6.2.3. Surface Water Flow

The water body of interest is a river system. In a preliminary exposure assessment, the project objectives indicate the use of a steady-state analysis of the flow system because the data are limited. A one-dimensional approach is appropriate for the system. Several different options may be considered at this point. The most conservative option would use the estimated or recorded low-flow rates (a reasonable worst-case condition); a somewhat less conservative analysis may use a yearly average flow rate. The annual variablity in the flow rate, along with some sensitivity studies, should provide some judgment on the choice of model. The surface water flow analysis may include an analytical estimate of velocity (i.e., Manning's equation); a computer-based model; or field measurements of velocity and travel time information between reaches. If a computer model is used, the HEC-2 model would be an appropriate choice for the river system.

6.2.4. Surface Water Contaminant Transport

Although the contaminant is a nonpoint source, the site is relatively small and could be represented as a point source, since the user is more interested in the impact of contaminant concentrations a considerable distance downstream. The contaminant from the surface runoff will be highly variable, only occurring during rainfall periods. If a continuous nonpoint source is used at the annual average rate estimated from the MRI loading function, the concentration estimates will underpredict the peak concentrations.

A conservative analysis could be performed by using a model with transient source terms and apportioning the MRI annual loading term between a few events. The first option to consider would be the most conservative analysis; that is, to use the entire annual contaminant loading in a single event. If the results indicate a potential exposure problem, the next step would be to represent the surface runoff contaminant loadings as a series of separate events. An analysis of rainfall and streamflow records may provide some guidance in the apportioning of annual loading terms into individual events.

Since the project objectives are to perform a preliminary exposure assessment, a one-dimensional contaminant transport model is the most appropriate. The model selected should consider advection, and particle settling and transport, as dominant processes in the analysis. The contaminants, such as the heavy metals, tend to adsorb to the sediments, and the sorption process should be considered. The most relevant degradation and transformation processes in the study are hydrolysis, volatilization, and biodegradation. For a conservative analysis, the rate constants associated with these attenuation mechanisms should be conservative (longer half-life), so that the results overpredict concentration levels.

The models that fit the selection criteria process include WASTOX, TOXIWASP, CHNTRN, HSPF, and SERATRA. These models incorporate the transient nature of the contaminant. All of these models are fairly complex, and the number of input parameters and detailed description are more than may be necessary for the preliminary exposure assessment. Successful application of the models in a short time frame may not be possible.

Another option is to use an analytical solution to the transient advection dispersion equation with a first-order decay rate. A first-order decay rate must include all of the degradation and transformation processes, along with

the sorption mechanism for removing dissolved pollutants from the water column. Multiple sources may be superimposed in time if necessary. This approach is probably the most consistent with the defined project objectives, and may also be the only approach that may be completed within the time constraints. The concentration of dissolved and adsorbed fractions in the water column may be calculated based on the partition coefficient and suspended sediment concentration. Details of the formulation, along with particle settling as an effective decay term, are described by Delos et al. (1984). An appropriate analytical solution for one-dimensional advection, dispersion, and decay was provided in Fischer et al. (1979):

$$C_T(x,t) = \frac{M_I}{A\sqrt{4\pi Dt}} \exp - \left\{\frac{(X-Ut)^2}{\sqrt{4Dt}}\right\} K_T t \qquad \text{(Eq. 6-1)}$$

where

C_T is the total concentration (dissolved and adsorbed forms) in the water column (M/L3),

X is the downstream distance (L),

t is time (T),

M_I is the mass input of contaminant (M),

A is the cross-sectional area of the river (L^2),

D is the longitudinal dispersion coefficient (L^2/T)

U is the average velocity (L/T),

K_T is the total first-order decay coefficient for the dissolved and adsorbed fractions, and particulate adsorbed settling is represented as an effective decay term (1/T).

The following is a flow chart of the model selection process just described. This material is included to show how the selection process shown in Table 5-1 may be used as a form of a worksheet.

I. INITIAL ANALYSIS

A. Objectives: Preliminary exposure assessment of contaminant concentration in water column; dilution calculation indicates potential problem. Limited resources are presently available, and a screening analysis is necessary.

B. Contaminant Source: Runoff from recycling plant: chromium, lead, mercury, trichloroethylene, phenol, benzene, toluene.

C. Important Processes: Sorption, volatilization, hydrolysis, biodegradation.

II. NONPOINT SOURCE RUNOFF

A. Land Use: Open urban area.

B. Time Characteristics: Annual (based on screening level objectives).

C. Space Characteristics: One area 20 acres in size.

D. Processes: Sorption and erosion.

E. Model Selection: MRI nonpoint source loading functions.

III. SURFACE WATER FLOW

A. Type of Water Body: Stream river system.

B. Stratification: Not applicable.

C. Time: Steady state, use low-flow condition for conservative analysis.

D. Dimensionality: One-dimensional for stream and river.

E. Model Choice: Analytical, Manning formula.

IV. SURFACE WATER CONTAMINANT TRANSPORT

A. Source Type: Distributed runoff, but point source will be adequate.

B. Time: Source term is strongly variable; transient analysis is needed.

C. Dimensionality: One-dimensional mixing should be nearly uniform at the downstream distances of concern.

D. Mixing and Transport: Advection primarily; longitudinal dispersion secondarily.

E. Sediment Contaminant Interactions: Sorption.

F. Processes: Volatilization, hydrolysis, and biodegradation.

G. Model Selection: The transient models in Table 5-3 (WASTOX, TOXIWASP, HSPF, CHNTRN, SERATRA) are more complex than required for the preliminary analysis. Instead, a one-dimensional analytical solution, Equation 6-1, is chosen, representing transient source terms (through superposition), advection, dispersion, and combined first-order decay rate to represent all attenuation mechanisms.

6.3. DETAILED SITE-SPECIFIC ANALYSIS

The objectives of the study are to estimate the long-term accumulation and fate of heavy metals and organic contaminants in the bed sediments and to predict the concentration in the water column. The results of the modeling study will have some impact on the decision to perform or require more cleanup work at the site. In addition, the modeling study could indicate potential risk to the general public via the contaminants found at the site. Therefore, the detailed site-specific analysis may impact the decision to spend several millions of dollars for additional cleanup work. The detailed site-specific analysis should have lower uncertainties in the modeling results.

As with the preliminary analysis, the primary interests are the potential threat to drinking water supplies and accumulation in fish. The source of contaminants is surface runoff from the closed recycling facility. The specific contaminants to be analyzed are heavy metals such as chromium, lead, and mercury; and organics such as trichloroethylene, phenol, benzene, and toluene. Reviewing data presented in Callahan et al. (1979), the following processes are considered to be important for the constituents of interest: sorption, volatilization, hydrolysis, and biodegradation.

6.3.1. Selection of a Nonpoint Source Runoff Model

The land area is identified as an urban area that is relatively open and is adjoined by commercial and residential areas. Based on the defined objectives of a detailed analysis, a short time scale on the order of minutes to days is necessary. The spatial characteristics of the area are that it is 20 acres in size and bounded on one side by a stream. It is assumed that the dominant mechanism for transporting the contaminants from the land area to the stream is particulate sorbed erosion. The contaminants may also be entering the stream through the discharge of contaminated groundwater. Measurements of contaminant concentrations in the groundwater and the stream during low-flow periods may be necessary. The highly transient nature of the surface runoff can only be described with a continuous simulation model, and the timing of loading terms to the stream will be important in relation to various sedimentation processes. The appropriate group of models satisfying the above criteria include: HSPF, ARM-II, ACTMO, and CREAMS.

6.3.2. Surface Water Flow

The water body of interest is a stream-river system. The defined objectives of the study, and the relationship between the timing of the source term, flow rate, and sedimentation processes, indicate that a transient analysis of

the flow system is necessary. A one-dimensional approach is appropriate for the river. The group of models which satisfy the above criteria include CHNHYD, HEC-6, SEDONE, HSPF, and DWOPER. The sedimentation capabilities of SEDONE and HSPF, in addition to the nonpoint source runoff capabilities of HSPF, should be considered in this choice.

6.3.3. Surface Water Contaminant Transport

The small area of nonpoint source runoff may be represented as a point source, since we are interested in concentrations a considerable distance downstream. A transient analysis is necessary to describe the source terms and flow conditions. A one-dimensional analysis is appropriate, and the important processes to consider are advection and particle settling and transport. The scouring, deposition, and burial of sediments may also be very important, depending on the sediment load of the stream and river. The contaminants do adsorb to sediments, and the sorption process is considered to be important. The important degradation and transformation processes are identified as hydrolysis, volatilization, and biodegradation.

The initial group of models which fit the general criteria include: WASTOX, TOXIWASP, CHNTRN, HSPF, and SERATRA. The MEXAMS model is the only model with the capability for analyzing the complex interactions of metals, but it does not handle the transient source terms and flow conditions. The HSPF model may be the best choice because of the combined ability to simulate nonpoint source runoff, flow characteristics, and the resulting transport and fate of contaminants. The MEXAMS model may also be useful as an additional tool, under a steady-state simplification, to assess the relative importance of the different interactions associated with the fate of metals. A steady-state simplification appropriate for the MEXAMS model might be identified through examination of the transient results from another model. A time frame may be

selected on the basis of a critical period where the potential risk is highest and the source terms and flow conditions assumed to be constant at those conditions. The model selection process just described is summarized in the following flowchart.

I. INITIAL ANALYSIS

A. Objectives: Detailed analysis of contaminant concentration in water column, and accumulation in bed sediments. Dilution calculation, preliminary exposure assessment, and field measurements indicate contamination problem. Available resources do not pose a limiting constraint, and uncertainty in model predictions should be minimized.

B. Contaminant Source: Runoff from recycling plant: chromium, lead, mercury, trichloroethylene, phenol, benzene, toluene.

C. Processes: Sorption, volatilization, hydrolysis, biodegradation.

II. NONPOINT SOURCE RUNOFF

A. Land Use: Open urban area.

B. Time Characteristics: Continuous simulation necessary; event simulation may also be useful.

C. Space Characteristics: One area, 20 acres in size.

D. Processes: Sorption and erosion.

E. Model Selection: HSPF, ARM-II, ACTMO, CREAMS.

III. SURFACE WATER FLOW

A. Type of Water Body: Stream river system.

B. Stratification: Not applicable.

C. Time: Timing between the source term, flow rate and sedimentation processes will be important. A transient flow analysis may be necessary.

D. Dimensionality: One-dimensional for stream and river.

E. Model Choice: CHNHYD, HEC-6, SEDONE, HSPF, DWOPER.

IV. SURFACE WATER CONTAMINANT TRANSPORT

A. Source Type: Distributed runoff, but point source will be adequate.

B. Time: Source term is strongly variable; transient analysis is needed.

C. Dimensionality: One-dimensional mixing should be nearly uniform at the downstream distances of concern.

D. Mixing and Transport: Advection primarily, longitudinal dispersion secondarily.

E. Sediment Contaminant Interactions: Sorption, sediment transport.

F. Processes: Volatilization, hydrolysis, and biodegradation.

G. Model Selection: WASTOX, TOXIWASP, HSPF, CHNTRN, SERATRA. The MEXAMS model may also be useful for examining the complex interaction of metals.

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8. REVIEW OF EXAMPLE SURFACE WATER MODELS

8.1. NONPOINT SOURCE RUNOFF MODELS

METHOD NAME: Midwest Research Institute (MRI) Nonpoint Source Loading Function

PURPOSE: The method is designed to be used for preliminary estimation of nonpoint source loading rates for urban and nonurban areas.

SOLUTION TECHNIQUE: The method is empirical and uses the Universal Soil Loss Equation to predict sediment erosion.

DESCRIPTION: The loading functions are useful as a "first cut" estimate of nonpoint source loading rates. Only the transport of sediment-attached constituents is considered (e.g., no dissolved contaminants). Various constituents are considered, including pesticides and heavy metals. The method is applicable to a single, small to large, catchment. Loading rates are estimated as annual averages. All processes throughout the study area are lumped together so that no spatial resolution is available.

INPUT: Catchment characteristics: location, size, and land use categories. USLE parameters: source area, rainfall, soil erodibility, slope length and gradient, land use practices, ground cover, and sediment delivery ratio.

OUTPUT: The results of the method include the average daily contaminant loading rates from each land use category, and 30-day maximum and 30-day minimum loading rates.

COMPILATION REQUIREMENTS:

Source Language: Not applicable
Hardware Requirements: Calculator
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Moderate.

TIME REQUIREMENTS: Low.

SOURCE: See documentation.

DOCUMENTATION/REFERENCES:

McElroy, A. D.; Chiu, S. Y.; Nebgen, J. W.; Aleti, A.; Bennett, F.W. (1976) Loading functions for assessment of water pollution from nonpoint sources. EPA-600/9-76-151. NTIS No. PB-253-325. U.S. Environmental Protection Agency, Washington, DC.

METHOD NAME: NPS

PURPOSE: The NPS model was developed to estimate nonpoint source pollutant loads in urban and rural areas.

SOLUTION TECHNIQUE: Empirical.

DESCRIPTION: The NPS model is a continuous simulation model that can be used to simulate nonpoint source pollutant loads. The hydrologic runoff portion of the model is based on the Stanford Watershed Model. The model does not incorporate decay or degradation of pollutants and is not applicable to nonconservative substances. The model does not include a channel routing routine and should not be used for land areas greater than about 2 square miles (although it could be coupled with a channel routing model).

A variety of watershed-dependent parameters are required, including various soil moisture capacity parameters (defined as storage zones). During a storm event, rainfall is partitioned between the storage zones. After the rainfall, water is transferred between the storage zones. The sediment processes are modeled as the detachment of fines and subsequent transport of fines.

INPUT: Hydrologic parameters: rainfall records, soil moisture capacity parameters (defined as various storage zones), snow pack characteristics, sediment loading parameters, land-use characteristics, and sediment accumulation and removal rates (for dry periods) for impervious areas.

OUTPUT: The output of the model includes hydrographs for storm events, sediment and pollutant loads and concentrations as a function of time, and dissolved oxygen concentrations and temperature.

COMPILATION REQUIREMENTS:

Source Language: IBM FORTRAN IV
Hardware Requirements: IBM 360
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Medium, weeks.

SOURCE:

Lee A. Mulkey
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, GA 30605

DOCUMENTATION/REFERENCES:

Donigian, A.S., Jr.; Crawford, N.H. (1976a) Modeling pesticides and nutrients on agricultural lands. EPA-600/2-76-043. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

Donigian, A.S., Jr.; Crawford, N.H. (1976b) Modeling nonpoint pollution from the land surface. EPA-600/3-76-083. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

METHOD NAME: Agricultural Runoff Model (ARM II)

PURPOSE: The Agricultural Runoff Model is a nonpoint source model that can be used to estimate pollutant loadings in agricultural areas.

SOLUTION TECHNIQUE: Empirical.

DESCRIPTION: ARM II is a continuous simulation model applicable to agricultural areas. The original basis of the model is the Stanford Watershed Model. The model can be used to simulate the transport of various pollutants from agricultural lands to streams. The model simulates runoff of water, sediments, nutrients, and pesticides for intervals of 5 or 15 minutes. The kinetics used to characterize degradation and transformation of pollutants are described by first-order rate equations. The model does not incorporate a channel routing routine and hence should not be used for land areas larger than 2 square miles (although it could be coupled with a channel routing model). A variety of watershed-dependent parameters are required, including soil moisture capacity parameters and snowmelt parameters.

INPUT: Hydrologic parameters: rainfall records; streamflow records (for calibration); soil moisture capacity parameters; snowmelt rates; snowpack characteristics; sediment loading parameters; and topography of land, surface, and soil type. Chemical parameters: pesticide degradation rates, adsorption/desorption coefficients; and nutrient reaction rates and storage parameters.

OUTPUT: The output of the model includes: Volume of water stored in watershed in various zones, volume of runoff, concentration of dissolved nutrients and pesticides in runoff, concentration of adsorbed nutrients and pesticides in runoff, amount of nutrients stored in soil and plant materials.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: Implemented on an IBM 370/160 and also on a Hewlett Packard 3000 Series II
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Medium, weeks.

SOURCE:

Lee A. Mulkey
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, GA 30605

DOCUMENTATION/REFERENCES:

Crawford, N.H.; Donigian, A.S., Jr. (1973) Pesticide transport and runoff model for agricultural lands. EPA-660/2-74-013. U.S. Environmental Protection Agency, Office of Research and Development, Washington, DC.

Donigian, A.S., Jr.; Crawford, N.H. (1976) Modeling pesticides and nutrients on agricultural lands. EPA-600/2-76-043. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

Donigian, A.S., Jr.; Davis, H.H., Jr. (1978) Agricultural Runoff Management (ARM) Model User's Manual: Versions I and II. EPA-600/3-78-080. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

Donigian, A.S, Jr.; Beyerlein, D.C.; Davis, H.H., Jr.; Crawford, N.H. (1977) Agricultural Runoff Management (ARM) Model: Version II, Refinement and Testing. EPA-600/3-77-098. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

METHOD NAME: AGRUN

PURPOSE: The AGRUN model is a nonpoint source model applicable to agricultural watersheds.

SOLUTION TECHNIQUE: Soil loss is estimated using the USLE, infiltration is based on Horton's equation, and streamflow is simulated using a finite-difference procedure.

DESCRIPTION: The AGRUN model consists of several compatible programs designed to simulate agricultural runoff, transport, and movement in the receiving stream. The USLE is used to compute the suspended solids in the runoff, and no decay of pollutants is incorporated. The model is designed as a single-event simulation model. The physical processes simulated by the model are overland flow, erosion, and channel flow. The model can simulate multiple catchments and dendritic channel systems. The model is a modification of the SWMM model.

INPUT: Precipitation data; geometry of catchments; soil parameters (depth of layers, permeability, field capacity, and saturation); channel geometry (cross-section data, length, slope, and Manning's n).

OUTPUT: The output of the model is the concentration of constituents in a river as a function of space and time.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: UNIVAC 1108
Mass Storage Requirements: 512K bytes of core

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Medium, weeks.

SOURCE:

Dr. Larry Roesner
Camp, Dresser and McKee Inc.
7620 Little River Turnpike
Annandale, VA 22003

DOCUMENTATION/REFERENCES:

Roesner, L.A.; Zison, S.W.; Monser, J.R.; Lyons, T.C. (1975) Agricultural Watershed Runoff Model for the Iowa-Cedar River Basins. Prepared by Water Resources Engineers Inc., under contract no. 68-01-0742, for the U.S. Environmental Protection Agency, Systems Development Branch, Washington, DC.

METHOD NAME: ACTMO

PURPOSE: The ACTMO model is a nonpoint source model applicable to agricultural areas.

SOLUTION TECHNIQUE: Empirical.

DESCRIPTION: The model is a continuous simulation model. The hydrologic analysis of the model is coupled with the USDA watershed model, USDAHL-74 (Holton, 1975). The model is applicable to agricultural areas with one or more catchments. The physical processes included in the model are downslope surface flow towards stream channel, subsurface infiltration, groundwater interflow, evapotranspiration, snow accumulation and melt, and erosion based on the Universal Soil Loss Equation. A variety of chemical processes are incorporated, including adsorption, degradation, mineralization, and plant uptake of agricultural chemicals. The model is designed primarily for the analysis of agricultural chemicals, fertilizers, and pesticides.

INPUT: Watershed characteristics: slope, length, width, soil erodibility, ground cover, management practices, soil layers, and subsurface characteristics. Chemical data: date of application, application rate, absorption coefficients, breakdown coefficient, mixing depth, and preference for size fractions. Soil characteristics: field capacity, porosity, texture, and dispersion factor. Hydrologic data: rainfall, runoff, infiltration, and soil moisture. Erosion data: erosion rates, sediment deposition, and sediment texture fraction of area in rills and rill depth.

OUTPUT: The output of the model includes streamflow hydrograph, watershed erosion, quantity of chemicals in runoff, and quantity of chemicals in each model zone.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: The model is operational on an IBM 360 or 365 and UNIVAC 1108 computers
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Medium, weeks.

SOURCE:

Agricultural Research Service
U.S. Department of Agriculture
Hyattsville, MD

DOCUMENTATION/REFERENCES:

Frere, M.H.; Onstad, C.A.; Holtan, H.W. (1975) ACTMO: an agricultural chemical transport model. Publication No. ARS-H-3. U.S. Department of Agriculture, Agricultural Research Service, Hyattsville, MD.

Holtan, H.W.; Stiltner, G.W.; Henson, W.H.; Lopez, H.C. (1975) USDAHL-74: revised model of watershed hydrology. Technical Bulletin No. 1518. U.S. Department of Agriculture, Agricultural Research Service, Hyattsville, MD.

METHOD NAME: CREAMS

PURPOSE: The CREAMS model is a nonpoint source model that may be used to estimate pollutant loadings from agricultural areas.

SOLUTION TECHNIQUE: Empirical.

DESCRIPTION: The CREAMS model structure consists of three major components: hydrology, erosion/sedimentation, and chemistry. The hydrology component estimates the volume and rate of runoff, evapotranspiration, soil moisture content, and percolation. Two options are included for the estimation of runoff: 1) Soil Conservation Service curve number method, and 2) infiltration capacity based on the Green and Ampt equation. The first method is useful when only daily precipitation data are available, and the second is used when more detailed (hourly) data are available.

The erosion/sedimentation portion of the model considers the processes of soil detachment, transport, and deposition. The detachment of soil is modeled by a modified form of the USLE. The sediment transport is dependent upon the smaller of: 1) transport capacity or 2) detached sediments available for transport. If the transport capacity is exceeded, deposition occurs. A critical shear stress is used to define erosion within channels. Deposition of coarse-grained particles occurs as a result of reduced flow velocity in ponded areas.

The chemistry portion of the model considers nutrients and pesticides. The transport of soluble and sediment-attached chemicals is evaluated. Interaction between plants and chemicals within the root zone is also considered.

The model is designed to require a bare minimum of calibration parameters and is intended to be used for comparison of different management and land use strategies. The spatial scale of the model is intended to be the size of an agricultural field.

INPUT: Precipitation records, SCS curve number of infiltration parameters, USLE parameters, partition coefficients (for different chemicals), and decay coefficients.

OUTPUT: The output of the model includes surface runoff, erosion, sediment delivery to water body, and chemical concentration in the sediments and in the soil system.

COMPILATION REQUIREMENTS:

Source Language: Fortran
Hardware Requirements: Unknown
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Moderate.

TIME REQUIREMENTS: Medium, weeks.

SOURCE:

Walter G. Knisel
U.S. Department of Agriculture
Southeast Watershed Research Laboratory
Tifton, Georgia 31793

DOCUMENTATION/REFERENCES:

Knisel, W.G., ed. (1980) CREAMS: a field scale model for chemicals, runoff, and erosion from agricultural management systems. Conservation Report No. 26. U.S. Department of Agriculture, Science and Education Administration, Washington DC.

Svetlosanov, V.; Knisel, W.G., eds. (1982) European and United States Case studies in application of the CREAMS Model. Report No. CP-82-S11. International Institute for Applied Systems Analysis.

METHOD NAME: SWMM

PURPOSE: The SWMM model is designed to simulate nonpoint source runoff, primarily from urban areas.

SOLUTION TECHNIQUE: Some processes in the model are represented empirically, while others are represented by finite difference formulations.

DESCRIPTION: The SWMM model is an extensive program that models the rainfall/runoff cycle in urban areas in a comprehensive manner. The model is a continuous simulation model. Some methods for calculating infiltration rates are incorporated. The model is capable of simulating multiple catchments and dry-weather accumulation of particulate matter. Flow routing is calculated including storage and backwater effects. Conventional pollutants are simulated, as are arbitrary conservative substances. Erosion is simulated with the USLE.

INPUT: Precipitation data and other meteorological data; channel/pipe geometry and characteristics; properties of catchments (geometry, slope, roughness, infiltration parameters, impervious areas, and storage); USLE parameters; and parameters defining deposition ratio and washoff functions.

OUTPUT: The output of the model includes hydrographs and pollutographs at different points within the system.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: Applied on variety of mainframe computers
Mass Storage Requirements: 350K bytes of core

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Long, months.

SOURCE:

Tom Barnwell
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, GA 30613

DOCUMENTATION/REFERENCES:

Huber, W.C.; Heaney, J.P.; Nix, S.J.; Dickinson, R.E.; Polmann, D. (1982, June) Storm Water Management user's manual: Version III. EPA-600/2-84-109A. U.S. Environmental Protection Agency, Cincinnati, OH.

Torno, H.C. (1980) Proceedings, Stormwater Management Model (SWMM) user's group meeting, January 10-11, 1980. EPA 600/9-80-017. U.S. Environmental Protection Agency, Washington, DC.

8.2. SURFACE WATER FLOW MODELS

CODE NAME: HEC-2

PURPOSE: The HEC-2 program is designed to calculate the water surface profile in rivers for a steady flow discharge.

DIMENSIONALITY: One-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model based on a finite difference formulation of the governing differential equation.

DESCRIPTION: The model is a one-dimensional representation of the continuity equation coupled with the conservation of energy equation. Friction losses are calculated with the Manning equation. Various energy loss terms are included to account for expansion and contraction of the flow area, and obstruction by bridge piers. The solution algorithm starts at the bottom reach and solves the nonlinear energy equation iteratively, one reach at a time, moving upstream. The roughness parameter, Manning's n, may vary at each cross-section and may also be calculated directly for each reach if discharge and water surface elevation are available at each reach.

INPUT: Geometric data (channel areas, reach lengths); roughness coefficient, Manning's n; flow rate; tributary inflows; and downstream water surface elevation.

OUTPUT: The output of the model includes the water surface profile and velocity at each cross-section.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: The program has been implemented on various systems including CDC 7600, UNIVAC 11087, IBM 360, and Honeywell 635
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Moderate.

TIME REQUIREMENTS: Medium, week(s).

SOURCE:

Hydrologic Engineering Center
U.S. Army Corps of Engineers
Davis, CA

DOCUMENTATION/REFERENCES:

U.S. Army Corps of Engineers. (1973, Oct.) HEC-2: water surface profiles: user's manual. Hydrologic Engineering Center, Davis, CA.

CODE NAME: CHNHYD

PURPOSE: A hydrodynamic model for simulating flows and water surface elevation in stream/river networks.

DIMENSIONALITY: One-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model based on an integrated compartment formulation. Time integration may be performed explicitly or implicitly.

DESCRIPTION: The CHNHYD model is based on the conservation of mass and momentum equations. The conservation equations are represented using the integrated compartment method (ICM) (Yeh, 1981). The method combines the advantages of finite difference, finite element, and compartment analysis techniques. Friction losses are represented using a Manning formulation. Wind stresses at the water surface are also incorporated. Very general forms of boundary conditions are incorporated so that the model may be applied to a wide variety of situations. Networks or branching of channel systems can be analyzed.

INPUT: Geometry and grid definition; roughness coefficient, Manning's n; wind stress parameters; initial conditions: flow rates and water surface profile; boundary conditions: flow rate, water surface.

OUTPUT: The output of the model includes the velocity and water surface elevation at each reach of river system at each time step.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: IBM 3033
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Moderate, weeks.

SOURCE:

G. T. Yeh
Environmental Sciences Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 33830

DOCUMENTATION/REFERENCES:

Yeh, G.T. (1981) ICM: an integrated compartment method for numerically solving partial differential equations. ORNL-5684. Oak Ridge National Laboratory, Oak Ridge, TN.

Yeh, G.T. (1982) CHNHYD: a channel hydrodynamic model for simulating flows and water surface elevations in a stream/river network. ORNL-5701. Oak Ridge National Laboratory, Oak Ridge, TN.

CODE NAME: HEC-6

PURPOSE: The HEC-6 program is designed to calculate the water surface profile and the stream bed profile. Sediment load, water velocity, and water depth are calculated.

DIMENSIONALITY: One-dimensional.

SOLUTION TECHNIQUE: The model is a transient numerical model based on a finite difference formulation.

DESCRIPTION: The model is a one dimensional representation of the continuity equation coupled with the conservation of energy equation. Friction losses are calculated with the Manning equation. The time integration is performed using an explicit integration scheme. The sediment transport is modeled by the continuity equation coupled with empirical equations for transport capacity and erodibility. The model is only applicable to subcritical flows. No mathematically rigorous stability criteria are developed; however, rule-of-thumb criteria are suggested. The flow rate is constant, but changes in stream bed may change velocities.

INPUT: Geometric data (channel areas, reach lengths); roughness coefficient, Manning's n; flow rate; tributary inflows; concentration of suspended and bed sediments; unit weight of sediments; and water temperature.

OUTPUT: The output of the model includes the water surface profile, the stream bed profile, and the concentration of suspended sediments in each reach of the system.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: CDC 7600 and UNIVAC 1108
Mass Storage Requirements: 65K words of central memory and 500K words of extended memory

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Extensive, months.

SOURCE:

Hydrologic Engineering Center
U.S. Army Corps of Engineers
Davis, CA

DOCUMENTATION/REFERENCES:

U.S. Army Corps of Engineers. (1977, Mar.) HEC-6: scour and deposition in rivers and reservoirs; user's manual. Hydrologic Engineering Center, Davis, CA.

CODE NAME: SEDONE

PURPOSE: The SEDONE model is a transient model for simulating hydrodynamic flow and sediment transport in rivers and estuaries.

DIMENSIONALITY: One-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model based on a discrete element formulation of the conservation of mass.

DESCRIPTION: The primary emphasis of the SEDONE model is the simulation of sediment transport processes. The model also simulates the momentum and continuity equations for water. Three sediment layers are considered for each reach of a stream or estuary: 1) a stationary resident bed layer, 2) a bed slurry layer, and 3) a suspended sediment layer. Longitudinal transport is considered only in the upper two layers, and the bottom resident layer serves as a finite reservoir with vertical transport to the slurry bed layer. Different size classes of sediments with different physical properties are incorporated. The spatial discretization of the domain results in a system of coupled ordinary differential equations for the water surface elevation, flow rate, and sediment size concentration in the three layers. The ordinary differential equations are numerically integrated in time, using a Runge-Kutta-Gill integration scheme.

INPUT: Geometry and grid definition, stream flow, lateral inflows, physical properties of each sediment size class, precipitation, and tidal boundary.

OUTPUT: The output of the model includes the water surface profile, flow rates, and sediment concentrations for each size class in the three layers for each reach of the system.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: The model has been implemented on an IBM 360/91
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Extensive, months.

SOURCE:

DOCUMENTATION/REFERENCES:

Hetrick, D.M.; Eraslan, A.H.; Patterson, M.R. (1979) SEDONE: a computer code for simulating tidal transient, one-dimensional, hydrodynamic conditions and three-layer, variable sediment concentrations in controlled rivers and estuaries. NUREG 6/CR-0430; ORNL/NUREG/TM-256. Oak Ridge National Laboratory, Oak Ridge, TN.

CODE NAME: DWOPER

PHYSICAL PROCESSES: A hydrodynamic model for simulating flow in rivers.

DIMENSIONALITY: Transient, one-dimensional.

SOLUTION TECHNIQUE: Numerical solution using an irregular finite difference grid. Time integration is performed implicitly.

DESCRIPTION: DWOPER is based on a one-dimensional form of the conservation of mass and momentum equations (St. Venant equations). The model can be used to simulate transient one-dimensional flow in river systems. The model is quite general in that it incorporates spatially variable physical parameters such as channel geometry, roughness parameters, lateral inflows, flow diversions, off-channel storage, local head losses, lock and dam operations, and wind stresses. The implicit time integration technique allows for the use of large time steps when appropriate. Additional features of the model include an automatic calibration procedure, internal to the model, whereby the roughness parameters in the friction slope term are automatically adjusted to minimize the difference between computed and observed stages. Data management routines are included to assist in the development of input parameters and the interpretation and display of output parameters.

CODE INPUT: River system configuration: channel configuration; cross-section geometry, initial roughness coefficients (Manning n), off-channel storage areas, and lateral inflows.

Initial conditions: estimated stage and discharge at each cross-section.

Boundary conditions: known stage or discharge at the upstream boundary as a function of time and stage or discharge hydrograph at downstream boundary.

CODE OUTPUT: Stage and discharge at each cross-section as a function of time.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: Small, Medium, and Large Storage sizes are available requiring 170, 235, 300K words (8 byte) of memory storage

EXPERIENCE REQUIREMENTS: Moderate, short courses are offered by the National Weather Service.

TIME REQUIREMENTS: Weeks.

SOURCE:

D. L. Fread
Hydrologic Research Laboratory
National Weather Service, NOAA
Silver Spring, MD 20910

DOCUMENTATION/REFERENCES:

Chen, Y.H.; Simons, D.B. (1975, Sept.) Mathematical modeling of alluvial channels. In: Modeling 75: symposium of modeling techniques. Vol. 1. American Society of Civil Engineers, pp. 466-483.

Fread, D.L. (1973a) Effect of time step size in implicit dynamic routing. Water Resources Bull. 9(2):338-351.

Fread, D.L. (1973b) Technique for implicit dynamic routing in rivers with major tributaries. Water Resources Bull. 9(4):918-926.

Fread, D.L. (1974, Mar.) Numerical properties of implicit four-point finite difference equations of unsteady flow. Technical Memorandum NWS HYDRO 18. National Oceanic and Atmospheric Administration, Washington, DC.

Fread, D.L. (1976) Flood routing in meandering rivers with flood plains. In: Rivers '76, Vol. I: symposium on inland waterways for navigation, flood control, and water diversions, held August 10-12, 1976, at Colorado State University. American Society of Civil Engineers, pp. 16-35.

Fread, D.L. (1978, Apr.) National Weather Service Operational Dynamic Wave Model. National Oceanic and Atmospheric Administration, Washington, DC.

Fread, D.L.; Price, R.K. (1975) Discussion of comparison of four numerical methods for flood routing. J. Hydraulics Div. ASCE 101(HY3):565-567.

Fread, D.L.; Smith, G.F. (1978) Calibration technique for one-dimensional unsteady flow models. J. Hydraulics Div. ASCE 104(July).

Fread, D.L.; Amein, M.; Fang, C.S. (1971) Discussion of implicit flood routing in natural channels. J. Hydraulics Div. ASCE 99(HY7):1156-1159.

CODE NAME: Dynamic Estuary Model (DYNHYD3)

PURPOSE: DYNHYD3 was developed to simulate hydrodynamic flow and contaminant transport and degradation in rivers and estuaries. The hydrodynamics program DYNHYD4 has been updated and linked to WASP3.

DIMENSIONALITY: One-dimensional (link-node two-dimensional)

SOLUTION TECHNIQUE: The model is a numerical model using the finite difference method to approximate the governing differential equations. The model is a one-dimensional model formulated in a "link node" manner so that some two-dimensional geometry may be represented by a series of channels and junctions.

DESCRIPTION: The model is a transient model based on conservation of momentum and continuity. The physical processes included in the model are tidal dynamics, river flow, and the advection and dispersion of contaminants. Various chemical processes are incorporated in the water quality portion of the model, including coupled and uncoupled reactions and first-order decay. A variety of chemical constituents are considered, including pesticides and heavy metals.

The time integration is performed explicitly; hence, an appropriate time step/grid size relationship must be chosen to avoid instabilities. Only constant sources of contaminants can be considered.

The hydrodynamic flow portion of the model can be run until a "dynamic steady state" condition is reached using the same tidal driving forces. Alternatively, the hydrodynamics can be run with variable inflows, wind, and tidal ranges. The tidally fluctuating velocities and water surface elevations are then used in the water quality simulation.

INPUT: Junction and channel geometry; friction coefficient (Manning's n); head water and tributary inflows; dispersion coefficients; rate constants for kinetic reactions; initial conditions (velocity, water surface elevation, concentrations); and boundary conditions (seaward tidal condition, source terms).

OUTPUT: The output of the model includes the velocity, water surface elevation, and contaminant concentrations as a function of space and time over the tidal cycle.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: IBM 370/168; DYNHYD3 is available on PC-compatible microcomputers
Mass Storage Requirements: Some disk storage, amount unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Extensive, months.

SOURCE:

R. B. Ambrose
U.S. Environmental Protection Agency
College Station Road
Athens, GA 30605

DOCUMENTATION/REFERENCES:

Ambrose, R.B.: Roesch, S.E. (1982, Feb.) Dynamic estuary model performance. Paper No. 16847. J. Environmental Engineering Div. ASCE 108(EE1):51-71.

Feigner, K.D.; Harris, H.S. (1970) Documentation report, FWQA Dynamic Estuary Model. U.S. Department of the Interior, Federal Water Quality Administration, Washington, DC.

Water Resources Engineers, Inc. (1974) Computer program documentation for the dynamic estuary model. U.S. Environmental Protection Agency, Systems Development Branch, Washington, DC.

CODE NAME: EXPLORE-I

PURPOSE: The EXPLORE-I model was developed to simulate hydrodynamics and water quality processes in water bodies (rivers, lakes, and estuaries).

DIMENSIONALITY: One-dimensional (link-node two-dimensional)

SOLUTION TECHNIQUE: The model is a numerical model using the finite difference technique. The model is a one-dimensional model formulated in a "link node" manner so that some two-dimensional geometry may be represented by a series of channels and junctions.

DESCRIPTION: The EXPLORE-I model consists of four separate computer codes: a hydraulic code for rivers and estuaries, a water quality code for rivers and estuaries, a hydrothermal code for thermally stratified reservoirs, and a water quality code for thermally stratified reservoirs. The hydraulic model is based on the conservation of momentum and mass (St. Venant equations). The river water quality model examines only the advection and degradation of contaminants; no dispersion term is included.

INPUT: Junction and channel geometry, friction coefficient (Manning's n), inflow and outflow, rate constants for kinetic reactions, initial conditions (contaminant concentrations), and boundary conditions (stage, discharge, contaminant concentration, and source term).

OUTPUT: The output of the model includes stage, discharge, and contaminant concentration at each node for each time step.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: The model is implemented on IBM 370 and Univac 1100 computers
Mass Storage Capacity: Disk storage 44K words

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: High, month(s).

SOURCE:

R. B. Ambrose
U.S. Environmental Protection Agency
Athens Environmental Research Center
College Station Road
Athens, GA 30613

DOCUMENTATION/REFERENCES:

Baca, R.G.; Waddel, W.W.; Cole, C.R.; Brandstetter, A.; Cearlock, D.B. (1973a) EXPLORE-I: a river basin water quality model. Prepared by Battelle Pacific Northwest Laboratories, Richland, WA, for the U.S. Environmental Protection Agency.

Onishi, Y. (1982) User's manual for EXPLORE-I: a river basin water quality module (hydraulic module only). EPA-600/3-82-054. U.S. Environmental Protection Agency.

CODE NAME: CAFE

PURPOSE: Two-dimensional hydrodynamics simulation in estuaries.

DIMENSIONALITY: Two-dimensional horizontal plane.

SOLUTION TECHNIQUE: The model is a numerical model that uses a finite element approximation to the governing partial differential equations.

DESCRIPTION: The two-dimensional, depth averaged model is based on the conservation of momentum and mass. The partial differential equations are incorporated in finite element form with triangular elements. The use of triangular elements are convenient for the description of irregular boundaries. The model assumes that the fluid density is independent of the velocity field. Friction is represented as an effective shear stress. The model incorporates wind stresses at the water surface.

INPUT: Geometry and grid definition; initial conditions for velocities and water surface elevation; boundary conditions, water surface elevations, and/or velocities; bottom friction coefficients; eddy viscosity coefficients; and wind magnitude and direction.

OUTPUT: Fluid velocities and water surface elevation as a function of space and time.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: CDC 7600
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: High, months.

SOURCE: See user's manual.

DOCUMENTATION/REFERENCES:

Pagenkopf, J.R.: Christodonlou, G.C.; Pearce, B.R.; Connor, J.J. (1976) A user's manual for Case I, a two-dimensional finite element circulation model. Report No. 217. Cambridge, MA: Massachusetts Institute of Technology, Department of Civil Engineering.

Wang, J.D.; Connor, J.J. (1975) Mathematical modeling of near coastal circulation. Report No. 200. Cambridge, MA: Massachusetts Institute of Technology, Department of Civil Engineering.

CODE NAME: WATFLO

PURPOSE: A hydrodynamic model for simulating flow in rivers and estuaries.

DIMENSIONALITY: Two-dimensional, horizontal plane.

SOLUTION TECHNIQUE: The model is a numerical model using the finite difference technique to approximate the governing differential equations.

DESCRIPTION: The model is a two-dimensional depth averaged model based on the couple equations describing conservation of momentum and mass. Time integration is performed using a multi-operational finite difference scheme. The domain of the system is represented on a staggered finite difference grid. The model is a modification of Leendertse's 2-D model; adaptations were performed by the Delft Hydraulics Laboratory. One important modification is a curvilinear coordinate transformation particularly well suited for the simulation of rivers.

The model does not include density effects, and friction is represented as an effective shear stress.

INPUT: Geometry and grid definition; bathymetry; friction coefficient (Chezy's C); initial conditions (water elevation and 2-D velocity field); and boundary conditions (inflows, water surface elevation, and or velocity).

OUTPUT: The output of the model includes the water surface elevation and the depth averaged X-Y velocity components.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: Unknown
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: High, months.

SOURCE: Available on contractual basis from

Charles E. Sweeney
Engineering Hydraulics Inc.
P. O. Box 3099
Redmond, WA 98052

(206) 881-7700

DOCUMENTATION/REFERENCES: Available from Engineering Hydraulics Inc., and

Leendertse, J.J. (1967) Aspects of a computational model for long-period water-wave propagation. RM-5294-PR. Santa Monica, CA: The Rand Corporation.

CODE NAME: Water Quality Simulation Model for Well-Mixed Estuaries and Coastal Seas (Leendertse-2D).

PURPOSE: A hydrodynamic and water quality model for simulating flow and contaminant transport.

DIMENSIONALITY: Two-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model using the finite difference technique to approximate the governing differential equations.

DESCRIPTION: The model is a two-dimensional, depth-averaged model based on the coupled equations describing the conservation momentum and mass (both fluid and contaminant). The time integration is performed using a multi-operational finite difference scheme. The domain of the system is represented by a staggered finite difference grid. The model is capable of simulating water flow and the advection and dispersion of contaminants in coastal seas and well-mixed estuaries.

The model does not include density effects or wind stress effects. Small scale velocity fluctuations are aggregated into the shear stress terms.

INPUT: Geometry and grid definition; bathymetry; friction coefficient (Chezy's C); dispersion coefficients; initial conditions (water surface elevation, X and Y velocity components, and contaminant concentrations); and boundary conditions (contaminant sources, inflows water surface and/or velocity, and tidal elevation).

OUTPUT: The output of the model includes the water surface elevation, depth averaged X and Y velocity components, and contaminant concentration as a function of space and time.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: Unknown
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: High, month(s).

SOURCE:

David Liu
Rand Corporation
Santa Monica, CA

DOCUMENTATION/REFERENCES:

Leendertse, J.J. (1967) Aspects of a computational model for long-period water-wave propagation. RM-5294-PR. Santa Monica, CA: The Rand Corporation.

Leendertse, J.J. (1970) A water quality model for well mixed estuaries and coastal seas. In: Principles of computation, Vol. I. RM-6230-RC. Santa Monica, CA: The Rand Corporation.

CODE NAME: A Three-Dimensional Model for Estuaries and Coastal Seas (Leendertse-3D).

PURPOSE: A model for simulating hydrodynamic flow and transport in estuaries and coastal seas.

DIMENSIONALITY: Three-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model using the finite difference technique to approximate the governing differential equations.

DESCRIPTION: The model is a three-dimensional model based on the coupled equations describing the conservation momentum and mass. The momentum equation is only represented in the X and Y directions, based on the assumption that the vertical accelerations (Z direction momentum equation) are much smaller than the acceleration due to gravity and may be neglected. The time integration is performed using an explicit finite difference scheme with the variables at each X-Y point over the vertical water column (Z direction) solved for implicitly to enhance stability. The domain of the system is represented by a staggered finite difference grid. The model is capable of simulating water flow and contaminant transport in coastal seas and well-mixed estuaries.

The model includes density effects and wind stress effects. The density variations are represented with an equation of state incorporating temperature and salinity changes. Wind stress at the water surface is represented as a quadratic function of the wind speed. Shear stress at the bottom is represented as quadratic function of the X and Y fluid velocity components.

INPUT: Geometry and grid definition; bathymetry; friction coefficient (Chezy's C); dispersion coefficients; initial conditions (water surface elevation, X, Y and Z velocity components, and contaminant concentrations); and boundary conditions (contaminant sources, inflows water surface and/or velocity, and tidal elevation).

OUTPUT: The output of the model includes the water surface elevation, X, Y and Z velocity components, and contaminant concentration as a function of space and time.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: IBM 360-91
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: High, months.

SOURCE:

David Liu
Rand Corporation
Santa Monica, CA

DOCUMENTATION/REFERENCES:

Leendertse, J.J.; Liu, S.-K. (1975) A three-dimensional model for estuaries and coastal seas. Vol. II: Aspects of computation. R-1764-OWRT. Santa Monica, CA: The Rand Corporation.

Leendertse, J.J.; Liu, S.-K. (1977) A three-dimensional model for estuaries and coastal seas. Vol. IV: Turbulent energy computation. R-2187-OWRT. Santa Monica, CA: The Rand Corporation.

Leendertse, J.J.; Alexander, R.C.; Liu, S.-K. (1973) A three-dimensional model for estuaries and coastal seas. Vol. I: Principles of computation. R-1417-OWRR. Santa Monica, CA: The Rand Corporation.

Leendertse, J. J., Liu, S.-K.; Nelson, A.B. (1975) A three-dimensional model for estuaries and coastal seas. Vol. III: The interim program, R-1884-OWRT. Santa Monica, CA: The Rand Corporation.

8.3. SURFACE WATER TRANSPORT MODELS

METHOD NAME: Water Quality Assessment Methodology (WQAM)

PURPOSE: The methodology was developed as a screening tool for the assessment of surface water quality in large basins.

DIMENSIONALITY: Zero-, one-, and two-dimensional.

SOLUTION TECHNIQUE: Analytical/empirical.

DESCRIPTION: The methodology is a collection of formulas, tables, and graphs for the preliminary assessment of water quality in large basins. Subject categories include: point and nonpoint waste load estimation, temperature, DO/BOD, nutrients, toxic chemicals, priority pollutants, and conservative and nonconservative constituents. Nonpoint source loading is based on the modified Universal Soil Loss Equation. Stream water quality is based on steady-state conservation of mass assuming plug flow. Water quality in lakes is based on a mass balance and empirical stratification relationship. The estuary water quality section is based on a tidal prism and/or fraction of freshwater analyses.

INPUT: Land use patterns, stream lengths, flow rates, reservoir volumes and depths, estuary salinity distributions, and point source loads.

OUTPUT: The output of the analyses is a steady-state concentration of the various constituents and pollutants subject to the loading rates defined.

COMPILATION REQUIREMENTS:

Hardware Required: Calculator

EXPERIENCE REQUIREMENTS: Low.

TIME REQUIREMENTS: Low, days.

SOURCE:

T. O. Barnwell
U.S. Environmental Protection Agency
Environmental Research Laboratory
Center for Water Quality Modeling
College Station Road
Athens, GA

DOCUMENTATION/REFERENCES:

Mills, W.B.; Dean, J.D.; Porcella, D.B.; Gherini, S.A.; Hudson, R.J.M.; Frick, W.E.; Rupp, G.L.; Bowie, G.L. (1982, Sept.) Water quality assessment: a screening methodology for toxic and conventional pollutants. Parts 1, 2, and 3. EPA-600/6-82-004a,b,c. U.S. Environmental Protection Agency, Washington, DC.

METHOD NAME: Simplified Lake/Stream Analyses (SLSA)

PURPOSE: SLSA is a screening model for the analysis of dissolved and sorbed steady-state concentration distributions in the water column and bed sediments of rivers and lakes.

DIMENSIONALITY: Zero- and one-dimensional.

SOLUTION TECHNIQUE: Analytical solution.

DESCRIPTION: SLSA can be used to analyze the steady-state advective transport of a pollutant; no dispersion term is incorporated. Degradation processes are represented by first-order rate constants, which are summed to yield an aggregate decay rate. Sediment suspension and exchange between the water column and the bed sediments are incorporated in this simplified modeling analysis. The sediment concentration suspended in the water column is a constant user-specified value. Only one reach of the river system is analyzed, assuming uniform flow and geometry characteristics. The model is a steady-state model with some "quasi-time varying" capabilities.

When applied to the analysis of rivers, the method is a one-dimensional analysis. When applied to the analysis of lakes, the method is a zero-dimensional (CSTR) analysis.

ASSUMPTIONS/LIMITATIONS: All decay kinetics are first-order. Dispersion is not considered. Bed sediment is assumed to be stationary and completely mixed. Only one particle size is considered. One single point source is considered. Only one river reach is considered, with no lateral inflows.

INPUT: Pollutant loading; flow rates, water and sediment depths, and length of reach; suspended solids in water column, sedimentation, and resuspension velocities; rate constants for kinetic reactions in water column and sediment distribution coefficients.

OUTPUT: The output of the model is the pollutant concentrations in the water column and in the bed sediments.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN, calculations are also simple enough for a calculator
Hardware Requirements: Suitable for microcomputer
Mass Storage Requirements: None

EXPERIENCE REQUIREMENTS: Low.

TIME REQUIREMENTS: Low, days.

SOURCE:

William Gullege
Chemical Manufacturers Association
2581 M Street, N.W.
Washington, DC 20037

DOCUMENTATION/REFERENCES:

HydroQual Inc. (1981) Analysis of fate of chemicals in receiving waters. Phase I. Prepared for Chemical Manufacturers Association, Washington, DC.

HydroQual Inc. (1982) Application guide for CMA-HydroQual chemical fate models. Prepared for Chemical Manufacturers Association, Washington, DC.

CODE NAME: MICHRIV

PURPOSE: MICHRIV is a steady-state model for simulating the transport of contaminants in the water column and bed sediments in streams and nontidal rivers.

DIMENSIONALITY: One-dimensional.

SOLUTION TECHNIQUE: Analytical computer model.

DESCRIPTION: MICHRIV can be used to analyze the steady-state advective transport of a pollutant; no dispersive term is incorporated. Degradation processes are represented as an aggregate first-order decay rate. The river can be segmented into successive reaches where characteristics are reasonably constant. The sediment concentration within the water column is a solution variable which is a function of the flow characteristics and sources. Since the model is based on an analytical solution, it is comparatively easy to set up and use.

ASSUMPTIONS/LIMITATIONS: All decay coefficients are first-order. Dispersion is not considered. Only one particle size is considered. This modeling analysis is only applicable to steady-state flow and loading conditions.

INPUT: System geometry, flow rates, loading rates of pollutants and particulates, partition coefficients, first-order decay coefficients, and sediment/water exchange parameters.

OUTPUT: The output of the model includes the pollutant concentration, in dissolved and particulate forms, as a function of distance from the source. The suspended sediment concentration is also predicted.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: Suitable for microcomputer
Nass Storage Requirements: None

EXPERIENCE REQUIREMENTS: Low.

TIME REQUIREMENTS: Moderate, weeks.

SOURCE:

Bill L. Richardson
U.S. Environmental Protection Agency
Environmental Research Station - Duluth
Large Lakes Research Station
Grosse Ile, MI 48138

DOCUMENTATION/REFERENCES:

DePinto, J.V.; Richardson, W.L.; Rygwelski, K. (1984) Technical guidance manual for performing waste load allocation. EPA-440/4-84-022. U.S. Environmental Protection Agency, Washington, DC.

CODE NAME: Chemical Transport and Analysis Program (CTAP)

PURPOSE: CTAP is a multi-dimensional, steady-state model for the analysis of dissolved and sorbed concentration distributions in the water column and bed sediments of rivers, lakes, and estuaries.

DIMENSIONALITY: One-, two-, or three-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model in finite difference form. The numerical approximation is formulated in compartments so that it may be applied to one-, two-, or three-dimensional problems.

DESCRIPTION: The CTAP model simulates the hydrologic transport and degradation of contaminants in water systems. The hydrologic transport processes included are advection and dispersion. Degradation is represented by first-order reaction kinetics for photolysis, oxidation, hydrolysis, and biodegradation. Decay rate coefficients are supplied by the user and summed to form an aggregate decay rate. Sorption of dissolved contaminants to sediments is incorporated as an equilibrium process. Sedimentation processes included in the model are bed movement, settling, suspension, burial, and diffusive exchange between bed sediments and dissolved contaminants. Five different particle sizes are accounted for, and multiple source terms are allowed.

ASSUMPTIONS/LIMITATIONS: Degradation is limited to first-order kinetics. The flow field must be defined externally via direct measurements or a hydrodynamic simulation model. Nonpoint sources are not incorporated. Steady-state analysis is limited to continuous sources.

INPUT: Geometry and grid definition, fluxes between compartments and dispersion coefficients, pollutant loadings, sediment fluxes between compartments and dispersion coefficients, sediment loadings, equilibrium distribution coefficients for each sediment category, kinetic reaction coefficients.

OUTPUT: The output of the model is the spatial distribution of chemical concentrations in dissolved and particulate forms. Concentrations are described for both the water column and the bed sediments.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: The model has been implemented on various computers including IBM 360/370, Univac 1108, CDC 6600, PDP 11/70, VAX 11-750, 11-780, IBM 1130.
Mass Storage Requirements: Some subroutine overlay with disk scratch files may be necessary to implement the model on minicomputers (without virtual memory).

EXPERIENCE REQUIREMENTS: Moderate.

TIME REQUIREMENTS: Moderate, weeks.

SOURCE:

William Gulledge
Chemical Manufacturers Association
2581 M Street, N.W.
Washington, DC 20037

(202) 887-1183

DOCUMENTATION/REFERENCES:

Games, L. (1981) Practical applications and comparisons of environmental exposure assessment models. Presented at the American Society for Testing and Materials Sixth Symposium of Aquatic Toxicology, St. Louis, MO.

HydroQual Inc. (1981) CTAP Documentation: Chemical Transport Analysis Program. Prepared for the Chemical Manufacturers Association, Washington, DC.

HydroQual Inc. (1982) Application guide for CMA-HydroQual chemical fate models. Prepared for the Chemical Manufacturers Association, Washington, DC.

CODE NAME: EXAMS

PURPOSE: Designed to evaluate the fate, exposure, and persistence of toxic chemicals in water systems where the concentrations of pollutants are at trace levels and the pollutant loading rates can be assumed to be steady state.

DIMENSIONALITY: One-, two-, or three-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model in finite difference form. The numerical approximation is formulated in compartments so that it may be applied to one-, two-, or three-dimensional problems.

DESCRIPTION: EXAMS can be used to simulate the hydrologic transport and biochemical transformation of toxic chemicals in the water environment. The hydrologic transport processes that are included are advection and dispersion. The transformation processes that are included in the model are photolysis, hydrolysis, biotransformation, oxidation reaction, and sorption with sediments and biota. In addition, volatilization at the water-air interface is also incorporated. Secondary daughter products and subsequent degradation of those products are considered.

The model is not designed to evaluate the contaminant concentration from pollutant problems such as spills of toxic chemicals. This limitation is the result of two assumptions incorporated in the model: 1) the steady flow field may not adequately describe the hydrologic transport processes associated with a large spill; and 2) the transformation processes included in the model assume that a toxic contaminant does not change the environmentsl factors that govern its transformation; in other words, the contaminants are present at trace levels.

ASSUMPTIONS/LIMITATIONS: The important assumptions/limitations are: steady-state or monthly-varying loading and flow field; the hydrodynamic flow field is determined externally from the model and input as vectors of flux and dispersion between compartments; chemicals in the water system are at trace levels and hence do not change the characteristics of the water system responsible for the transformation of the chemicals; sorption/desorption processes are assumed to be at equilibrium within each compartment; and the chemicals within any compartment are assumed to be uniformly mixed and homogeneous throughout the given compartment.

INPUT: System geometry (volumes, areas, and transport pathways between zones); hydrologic parameters (fluxes between zones, rainfall, evaporation rates, entering stream flows, nonpoint source loads, sediment loads, and groundwater flows); transformation parameters (sediment and biota sorption, volatilization, photolysis, oxidation, hydrolysis, and biotransformation); and environmental parameters (temperature, wind speed, pH, solar insulation, and scattering).

OUTPUT: The output of the model is the concentration of the pollutant of interest in the water, sediment, and biota for each zone. In addition, the concentrations of any daughter products due to transformations are included.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: The model has been implemented on various computer systems including IBM 370, CDC Cyber, PDP 11, HP 3000, and PC-compatible microcomputers.
Mass Storage Requirements: 2.5K words

EXPERIENCE REQUIREMENTS: Moderate.

TIME REQUIREMENTS: Moderate, weeks.

SOURCE:

Lawrence A. Burns
U.S. Environmental Protection Agency
Athens Environmental Research Laboratory
College Station Road
Athens, GA 30613

DOCUMENTATION/REFERENCES:

Burns, L.A.; Cline, D.M.; Lassiter, R.R. (1982) Exposure Analysis Modeling System (EXAMS): user manual and system documentation. EPA-600/3-82-023. U.S. Environmental Protection Agency, Athens, GA.

Burns, L.A.; Cline, D.M. (1985) EXAMS-II: Exposure Analysis Modeling System, Reference Manual for EXAMS-II. EPA-600/3-85-038. U.S. Environmental Protection Agency, Athens, GA.

CODE NAME: MEXAMS

PURPOSE: MEXAMS is a steady-state model designed to evaluate the fate and transport of metals in aquatic systems. The model is a linking of a geochemical model, MINTEQ, and EXAMS.

DIMENSIONALITY: One-, two-, or three-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model in finite difference form. The numerical approximation is formulated in compartments so that it may be applied to one-, two-, or three-dimensional problems.

DESCRIPTION: MEXAMS can be used to evaluate the hydrologic transport, biochemical transformation, and speciation of dissolved adsorbed and precipitated metals in the water environment. The chemical interactions are based on thermodynamic equilibrium relationships between the different species of the metal and pertinent water quality parameters. Several different adsorption algorithms are incorporated in the model. A thermodynamic data base for the following metals is incorporated in the model: arsenic, cadmium, copper, lead, nickel, silver, and zinc. The primary advantage of the MEXAMS model lies in its ability to represent the complex chemistry of metals in water bodies, particularly the effect of chemical speciation on adsorption and precipitation.

ASSUMPTIONS/LIMITATIONS: Steady-state loading and flow field; hydrodynamic flow field is determined externally; all chemical processes are considered to be equilibrium processes; the thermodynamic data base is limited to specific metals; and the chemicals within any given compartment are assumed to be uniformly mixed and homogeneous throughout.

INPUT: The first part of the input data is related to the EXAMS portion of the model and is described in the previous code description. The second part of the input data is related to the MINTEQ portion and is contained in a data base that goes with the model (but it is limited to the specific metals in the data base).

OUTPUT: The output of the model includes the concentration of the different metal species in different forms (dissolved, adsorbed, and precipitated) in each compartment of system.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: PDP 11/70 or HP 3000; MINTEQA1 available on PC-compatible microcomputers.
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: High, month(s).

SOURCE:

David Brown
U.S. Environmental Protection Agency
Athens Environmental Research Laboratory
Athens, GA 30613

DOCUMENTATION/REFERENCES:

Burns, L.A.; Cline, D.M.; Lassiter, R.R. (1982) Exposure Analysis Modeling System (EXAMS): user manual and system documentation. EPA-600/3-82-023. U.S. Environmental Protection Agency, Athens, GA.

Felmy, A.R.; Brown, S.M.; Onishi, Y.; Argo, R.S.; Yabusaki, S.B. (1982) MEXAMS: the Metals Exposure Analysis Modeling System. Contract No. 68-03-3089. Battelle Pacific Northwest Laboratories, Richland, WA.

Brown, D.S. (1987) MINTEQA1, an Equilibrium Metal Speciation Model: users manual. Final draft. U.S. Environmental Protection Agency, Athens, GA.

CODE NAME: TOXIWASP

PURPOSE: TOXIWASP is a transient model for simulating the transport and fate of toxic chemicals in water bodies. The model is basically a combination of the EXAMS and WASP models with additional sediment transport capabilities.

DIMENSIONALITY: One-, two-, or three-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model in finite difference form. The numerical approximation is formulated in compartments so that it may be applied to one-, two-, or three-dimensional problems.

DESCRIPTION: TOXIWASP can be used to simulate the hydrologic transport and biochemical transformation of toxic chemicals in the water environment. The hydrologic transport phenomena included are advection and dispersion. Various biochemical transformation processes are incorporated, including hydrolysis, biolysis, photolysis, oxidation, and volatilization. In addition, sorption onto biota and sediments are included. The transport of sediment includes advection, diffusion, and settling.

ASSUMPTIONS/LIMITATIONS: The important assumptions of the model are: the concentration in any compartment is completely mixed; sorption is treated as an equilibrium process; and the degradation rates for the different processes can be combined linearly to form a single degradation rate for particular chemicals in each segment. The explicit integration scheme is only conditionally stable, so that the time step must be chosen carefully. The hydrodynamic flow field must be determined externally.

INPUT: Geometry and grid definition; fluxes between zones; dispersion coefficients; initial conditions; boundary conditions; input loads; sediment properties (density, organic content, settling velocities, dispersion rates); chemical properties and rates (partition coefficients, hydrolysis, photolysis, and oxidation); and temperature, pH, light intensity, wind speed, and extinction coefficients.

OUTPUT: The output of the model is the contrations); and chemicals in the water and in the sediments as a function of space and time. Also output are some summary statistics and spatial plots of concentration.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN77
Hardware Requirements: The model has been implemented on PDP 11-70, IBM 370, and PC-compatible microcomputers.
Mass Storage Requirements: Disk storage 32K words; 512K and math coprocessor.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: High, month(s).

SOURCE:

Robert B. Ambrose, Jr.
U.S. Environmental Protection Agency
Athens Environmental Research Laboratory
Athens, GA 30613

DOCUMENTATION/REFERENCES:

Ambrose, R.B., Jr.; Hill, S.I.; Mulkey, L.A. (1983, Mar.) User's manual for the Chemical Transport and Fate Model (TOXIWASP), Version 1. EPA-600/3-83-005. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

Abrose, R.B. (1986, Mar.) WASP3, A Hydrodynamic and Water Quality Model (DYNHYD3), Model Theory, User's Manual and Programmer's Guide. EPA-600/3-86-034. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

CODE NAME: WASTOX

PURPOSE: WASTOX is a transient model for simulating the transport and degradation of toxic chemicals in water bodies.

DIMENSIONALITY: One-, two-, or three-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model in finite difference form. The numerical approximation is formulated in compartments so that it may be applied to one-, two-, or three-dimensional problems.

DESCRIPTION: WASTOX can be used to simulate the hydrologic transport and biochemical degradation of toxic chemicals in the aquatic environment. The hydrologic processes included are advection and dispersion. The model considers chemicals both in dissolved form and adsorbed to particulates. Kinetic processes are specified through subroutines that may be modified by the user. The model is similar to the TOXIWASP model, with some differences in the mechanisms for transport between bed sediments and the water column.

ASSUMPTIONS/LIMITATIONS: The important assumptions of the model are the concentration of contaminant in any compartment is completely mixed; and the degradation rates for the different processes can be combined to form a single degradation rate for the particular chemical in each compartment. The explicit integration scheme is only conditionally stable, so the time step and spatial resolution must be chosen carefully. The hydrodynamic flow field must be determined externally.

INPUT: Geometry and grid definition; fluxes between zones; dispersion coefficients; initial conditions; boundary conditions; rate constants for reaction kinetics; sediment characteristics; and temperature, pH, wind speed, and extinction coefficients.

OUTPUT: The output of the model is the pollutant concentration as a function of space and time. The contaminant concentration is given for both dissolved and particulate forms, along with the concentration with depth in the sediment.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN
Hardware Requirements: The model is implemented on a PDP 11-70
Mass Storage Requirements: Disk storage 25K words

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: High, month(s).

SOURCE:

John P. Connolly
Manhattan College
Bronx, NY 10471

DOCUMENTATION/REFERENCES:

Connolly, J.P.; Winfield, R.P. (1984, Aug.) A user's guide for WASTOX, a framework for modeling the fate of toxic chemicals in aquatic environments. Part 1: Exposure concentration. EPA-600/3-84-077. U.S. Environmental Protection Agency, Washington, DC.

CODE NAME: Channel Transport Model (CHNTRN)

PURPOSE: The CHNTRN model is a transient model for simulating the transport of sediments and contaminants in rivers and well-mixed estuaries.

DIMENSIONALITY: One-dimensional (possibly more with modifications).

SOLUTION TECHNIQUE: The model is a numerical model based on an integrated compartment formulation. A system of ordinary differential equations is formulated based on the conservation of mass for each compartment. Time integration may be performed explicitly or implicitly.

DESCRIPTION: The CHNTRN model is based on the conservation of mass and incorporates a variety of chemical kinetics, sediment transport, deposition, and scouring for sand, silt, and clay. The hydrologic transport processes included in the model are advection and dispersion. The model incorporates second-order kinetics using the EXAMS framework to account for hydrolysis, oxidation, photolysis, volatilization, biodegradation, and adsorption by biota. Sediment transport is represented in a mechanistic fashion, where the concentration and flux of sediments are unknown solution variables. The model is capable of simulating channel networks so that branching river and tributary systems may be analyzed. The integrated compartment formulation of the model may make modifications to the model, such as two- or three-dimensional simulations for lakes or estuaries, somewhat easier.

ASSUMPTIONS/LIMITATIONS: The important assumptions and limitations of the model are: the one-dimensional formulation limits the application to situations where parameters are well mixed vertically and laterally; hydrodynamic data must be specified externally (a companion code CHNHYD is available for hydrodynamic simulation); and extensive input data is required characterizing sediment sizes and chemical properties of the different sizes.

INPUT: Geometry and grid definition; hydrodynamic data, fluxes between compartments, dispersive coefficients; rate coefficients for photolysis, hydrolysis, oxidation, and biodegradation; pollutant sources and loads; sediment types and distributions; and temperature, wind speed, vapor pressure, and extinction coefficients.

OUTPUT: The output of the model includes: dissolved chemical concentration as a function of space and time, particulate concentration suspended in the water column and in bed sediments, and suspended sediment concentration and amount of sediment remaining in the bed.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN IV
Hardware Requirements: The model has been implemented on an IBM 3033
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Moderate, weeks.

SOURCE:

G. T. Yeh
Environmental Sciences Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 33830

DOCUMENTATION/REFERENCES:

Yeh, G.T. (1981) ICM: an integrated compartment method for numerically solving partial differential equations. ORNL-5684. Oak Ridge National Laboratory, Oak Ridge, TN.

Yeh, G.T. (1982) CHNTRN: a channel transport model for simulating sediment and chemical distribution in a stream/river network. ORNL-5882. Oak Ridge National Laboratory, Oak Ridge, TN.

CODE NAME: HSPF

PURPOSE: HSPF is a series of coupled computer codes designed to simulate: 1) watershed hydrology; 2) land surface runoff; and 3) the fate and transport of pollutants in receiving water bodies. The model is a transient model applicable to rivers and well-mixed (unstratified) reservoirs.

DIMENSIONALITY: The analysis of rivers is one-dimensional and the analysis of reservoirs is zero-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model in finite difference form with some empirical components.

DESCRIPTION: The HSPF model is a comprehensive model designed to simulate a wide variety of hydrologic and environmental phenomena affecting the fate and transport of pollutants. The hydrologic portions of the model include: 1) a watershed hydrology model similar to the Stanford Watershed Model; 2) a runoff model using algorithms similar to the Non-Point Source (NPS) model; and 3) a stream routing component using a kinematic wave approximation.

The analysis of sediment transport in the model is formulated in a mechanistic fashion. The sediment transport mechanisms incorporated in the model include settling, deposition, and scouring. Three particle sizes are incorporated in the model, generally corresponding to sand, silt, and clay. The adsorption/desorption processes are calculated separately for each particle size, suspended in the water column and in the bed sediment.

The degradation/transformation processes included in the model are: hydrolysis, photolysis, oxidation, volatilization, and biodegradation. The kinetic reactions are formulated as second-order processes. Secondary or "daughter" chemicals are also simulated; up to two daughter chemicals can be analyzed in a single simulation.

The model was initially formulated as the integration of several existing models, including: SWM, NPS, ARM, EXAMS, SERATRA, and HSP. Rather than identify the existing models as subroutines, the entire modeling framework was rewritten to make understanding and modifications to the program easier for users.

ASSUMPTIONS/LIMITATIONS: The important assumptions and limitations of the model are the one-dimensional formulation limits application of the model to river systems where pollutants are uniformly mixed both laterally and vertically; the kinematic wave formulation of flow in rivers is not applicable to rivers where the gradient is very small or where backwater effects are present; data requirements for the model may be quite extensive depending on the particular application; and the zero-dimensional representation of lakes assumes that pollutants are uniformly mixed throughout and that the lake is not stratified.

INPUT: The amount and types of input data are dependent on the particular options used in a given simulation. These data may include:

Time series inputs, including air temperature, precipitation, evapotranspiration, channel inflow, surface water and groundwater inflow, and wind movement;

Constant parameter inputs, including channel geometry, vegetative cover index, surface detention storage, groundwater storage volume, soil moisture content, overland flow slope, snow-pack data, infiltration index, and interflow index;

Land sediment factors: soil detachment coefficients, sediment influx, surface cover, and sediment washoff coefficient;

Soil temperature data: air temperature time series, slope, and intercept of land temperature to air temperature equation;

Dissolved gas in land water: ground elevation, interflow, and groundwater DO and CO2 concentrations;

Quality constituents associated with sediment: washoff potency factor and scour potency factor;

Quality constituents concentrations in interflow and groundwater;

Agrichemical quality constituent: solute leaching factors; soil layer depths; soil densities; and pesticide and nutrient sorption parameters, solubility factors, and degradation rates;

Impervious land quality factors: surface runoff removal rates, solids washoff coefficient, rate of solids placement and removal on surface, and overland flow-borne pollutant accumulation and storage rates; and

Reach and reservoir water quality characteristics, coefficients, and rates.

OUTPUT: HSPF output consists of multiple printouts, including system state variables, pollutant concentrations at a point versus time, and yearly summaries describing pollutant duration and flux. The model also includes a frequency analysis which provides a statistical summary of time-varying contaminant concentrations and provides the link between simulated instream toxicant concentrations and risk assessment.

COMPILATION REQUIREMENTS:

Source Language: FORTRAN77
Hardware Requirements: Originally developed on a HP 3000 system, the model has been installed on a wide variety of mainframe and virtual memory systems, and PC-compatible microcomputers.
Mass Storage Requirements: Twelve internal files are required and 128K bytes of instruction and data storage.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Moderate to high, weeks to months (depending on application).

SOURCE:

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U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, GA 30613

DOCUMENTATION/REFERENCES:

Donigian, A.S.; Imhoff, J.C.; Bicknell, B.R.; Kittle, J.L. (1984, June) Guide to the application of the Hydrological Simulation Program: FORTRAN (HSPF). EPA-600/3-84-065. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

Imhoff, J.C.; Kittle, J.L.; Donigian, A.S.; Johanson, R.C. (1984, June) Hydrological Simulation Program--FORTRAN (HSPF): User's manual for Release 8.0. EPA-600/3-84-006. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

Johanson, R.C.; Kittle, J.L. (1983) Design, programming, and maintenance of HSPF. J. Technical Topics in Civil Engineering 109(1):41-57.

Johanson, R.C.; Imhoff, G.C.; Davis, H.H. (1980) User's manual for Hydrological Simulation Program: FORTRAN (HSPF). EPA 600/9-9-80-015. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA.

CODE NAME: FETRA

PURPOSE: The FETRA model is a two-dimensional, depth averaged, transport model. The model simulates the transport of dissolved contaminants, sediments, and contaminants adsorbed by the sediments. The model is applicable to well-mixed estuaries, coastal seas, and some shallow lakes.

DIMENSIONALITY: Two-dimensional, horizontal plane.

SOLUTION TECHNIQUE: The model is a numerical model that uses a finite element approximation to the governing partial differential equations.

DESCRIPTION: The model is based on the general advection-diffusion equation with decay, source/sink terms, and appropriate boundary conditions. Three coupled submodels are included incorporating sediment transport, dissolved contaminant transport, and particulate contaminant transport. Sediment transport processes incorporated in the model include advection and dispersion, settling, deposition and erosion, and mixing from point and nonpoint sediment sources. Contaminant transport processes included in the model are advection, dispersion, adsorption/desorption by sediments, decay and biochemical degradation, and mixing of point and nonpoint contaminant sources.

INPUT: Geometry and grid definition; velocity field from a compatible flow simulation model; vertical dispersion coefficient; distribution coefficients (Kd) for each sediment; deposition and erosion rates for sediments; decay rate coefficients; particle settling velocity; particle density and diameter; critical shear stresses for bed scouring and sediment deposition; degradation and decay rates; initial conditions (dissolved contaminant concentrations, sediments, adsorbed contaminant concentrations, and bed conditions); and boundary conditions (sediment, dissolved and particulate contaminant concentrations at boundaries, and contribution from point and nonpoint sources).

OUTPUT: Concentration of contaminants as a function of space and time in dissolved and adsorbed form and location of sediment movement in bed and suspended in the water column.

COMPILATION REQUIREMENTS:

Source Language: FETRA is written in the FORTRAN preprocessor language FLECS. A standard FORTRAN IV version is available; however, it is difficult to interpret and the FLECS version is much easier to follow
Hardware Requirements: IBM, VAX, CDC-7600
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

SOURCE

Y. Onishi
Battelle, Pacific Northwest Laboratories
Richland, WA 99352

DOCUMENTATION/REFERENCES:

Onishi, Y.; Thompson, F.L. (1984) Mathematical simulation of sediment and radionuclide transport in coastal seas. Vol. 1: Testing of the sediment/radionuclide transport model, FETRA. Vol. 2: User's manual and computer listing for FETRA. NUREG/CR-2424; PNL-5088-1. Battelle Pacific Northwest Laboratory, Richland, WA.

CODE NAME: SERATRA

PHYSICAL PROCESSES: The SERATRA model can be used to simulate the transport of contaminants and sediments in rivers over a two-dimensional vertical plane.

DIMENSIONALITY: Two-dimensional.

SOLUTION TECHNIQUE: The model is a numerical model using the finite element method to approximate the governing differential equations.

DESCRIPTION: The model is based on the general advection-diffusion equation with decay, source/sink terms, and appropriate boundary conditions. Three coupled submodels are included which incorporate sediment transport, dissolved contaminant transport, and particulate contaminant transport. The sediment transport processes incorporated in the model include advection, dispersion, settling, deposition and erosion, and contributions from tributaries. The contaminant transport processes incorporated in the model include advection, dispersion, adsorption/desorption by sediments, decay and biochemical degradation, and mixing of point and nonpoint contaminant sources. Degradation processes included in the model are photolysis, oxidation, hydrolysis, biological decay, and volatilization at the water-air interface.

The model does not include a longitudinal diffusion term. A "downstream marching solution" is employed in the model; hence it is not applicable to tidal rivers, where the directions of flow may reverse.

ASSUMPTIONS/LIMITATIONS: The model represents a two-dimensional vertical plane, so that lateral variations across the stream are ignored (lateral variations may be important near point source and also in wide rivers); extensive input data is required characterizing sediment sizes and chemical properties of the various sizes; longitudinal dispersion is not considered, but variations in the longitudinal velocity over the vertical column can be incorporated; the flow field must be determined externally in a hydrodynamic simulation model or direct measurements.

CODE INPUT: The input to the model includes: geometry and grid definitions; discharge and depth of river; inflows from tributaries, overland runoff, and point and nonpoint sources; vertical dispersion coefficient; sediment sizes and densities; settling velocities; critical shear stress for erosion and deposition; erodibility coefficients; distribution coefficients for each sediment size; degradation and decay rates; initial conditions for sediments, dissolved, and particulate contaminants; and boundary conditions for sediments, dissolved, and particulate contaminants.

CODE OUTPUT: The output of the model includes the concentration of sediments, and dissolved and particulate contaminants as a function of space and time. In addition, changes in bed elevation and contaminant concentration in the bed sediments are provided.

COMPILATION REQUIREMENTS:

Source Language: SERATRA is written in the FORTRAN preprocessor language FLECS. A standard FORTRAN version is available; however, it is difficult to read (due to the FLECS translation), and the FLECS version is much easier to interpret.
Hardware Requirements: CDC and VAX
Mass Storage Requirements: Unknown

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

SOURCE:

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Richland, WA 99352

DOCUMENTATION/REFERENCES:

Onishi, Y.; Wise, S.E. (1982) User's manual for the Instream Sediment-Contaminant Transport Model SERATRA. EPA-600/3-82-055. U.S. Environmental Protection Agency, Washington, DC.

Onishi, Y.; Wise, S.E. (1982) Mathematical model, SERATRA, for sediment-contaminant transport in rivers and its applications to pesticide transport in Four Mile and Wolf Creeks in Iowa. EPA-600/3-82-045. U.S. Environmental Protection Agency, Washington, DC.

APPENDIX A

DEFINITION OF SYMBOLS

Symbol	Definition	Units
A	Average cross sectional area of river	L^2
C	Concentration of dissolved contaminants	M/L^3
C_f	Cover Factor	---
C_o	Initial concentration	M/L^3
C_T	Total concentration, dissolved and adsorbed	M/L^3
d	Depth	L
D	Dispersion coefficient	L^2/T
E_v	Vertical mixing coefficient	L^2/T
E_t	Transverse mixing coefficient	L^2/T
g	Acceleration of gravity	L/T^2
k	Rate coefficient	$1/T$
K_T	Total first order rate coefficient	$1/T$
K_f	Soil erodibility factor	T/L^2
K_p	Partition coefficient	M/M
l	Segment length	L
L_{gf}	Slope gradient factor	---
m	Mass discharge rate	M/T
M	Concentration of particulate matter	M/L^3
M_I	Initial mass of contaminant	M
P	Concentration of adsorbed contaminants	M/L^3
P_F	Erosion control practice factor	---
P_E	Peclet number	---
q	Vector of x,y,z velocity components	L/T

Symbol	Definition	Units
Q	Flowrate	L^3/T
Q_f	Freshwater inflow rate	L^3/T
Σr	Summation of reactions terms	$M/L^3/T$
R	Estuary Richardson number	---
R_f	Rainfall factor	M/T
R_p	Mass of chemical per unit mass of particulate	M/M
R_{xn}	Reaction number	---
s	Source/sink terms for dissolved contaminants	$M/L^3/T$
s_m	Source/sink terms for particulate matter	$M/L^3/T$
S	Channel slope	L/L
S_{gf}	Slope gradient factor	---
t	Time	T
t_A	Advection time	T
t_D	Diffusion time	T
t_T	Transformation time	T
ΣT	Summation phase transfer mechanisms	$M/L^3/T$
u^*	Shear velocity	L/T
U	Mean cross sectional velocity	L/T
V_a	Depth mean amplitude of current	L/T
V_t	Root mean square tidal velocity	L/T
W	Width	L
w_s	Settling velocity	L/T
x	Cartesian coordinate	L
X	Downstream distance	L

Symbol	Definition	Units
y	Cartesian coordinate	L
$Y(s)$	Annual sediment yield	M/L^2
z	Cartesian coordinate	L
∇	Del operator	$1/L$
α	Dimensionless empirical coefficient	---
ρ	Density	M/L^3
$\Delta\rho$	Difference in density	M/L^3

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