

CHAPTER 9

Use of Models in Nutrient Criteria Development

Model Identification and Selection
Model Classification
Use of Models for Nutrient Investigation
Management Applications

All models are wrong. Some models are useful.
(George E. P. Box)

9.1 INTRODUCTION

This chapter addresses the role of models in nutrient criteria development. It is closely linked to Chapter 5, which addresses database development, sampling designs, and monitoring. One system is said to model another when the observable variables in the first system vary in the same fashion as the observable variables in the second (NRC 2000). Chapter 7 of the NRC report goes on to state that models come in many forms. They may be empirically derived statistical relationships plotted on a graph, physical analogues (e.g., mesocosms) of the system of interest, analogues of different systems that have useful parallel relationships of observable factors (e.g., from physics, the flow of water through pipes to model the flow of electrons through an electrical circuit), or numerical models run on computers that are based on first principles or empirical relationships.

Environmental water quality models have several uses (e.g., reduce ecosystem complexity to a manageable level, improve the scientific basis for development of theory, provide a framework to make and test predictions, increase understanding of cause-and-effect relationships, and improve assessment of factor interaction). Reliable predictions stand out as a salient requirement because of the social and economic consequences if predictions are unreliable. Many times decisionmakers rely on models to guide their environmental management choices, especially when costly decisions are involved and the problem and solution involve complex relationships. This is exemplified by the decision of the Long Island Sound Hypoxia Management Conference (see Case Study for Long Island Sound). Generally, empirical and mathematical models are the most widely used models that statistically or mathematically relate nutrient loads or concentrations to important ecological response variables (e.g., dissolved oxygen deficiency, algal blooms and related decrease in water clarity, and loss of seagrasses). They both depend on the scientific robustness and accuracy of underlying conceptual models.

This chapter addresses both empirical and mathematical models. Considerably more space is devoted to mathematical models, because they are capable of addressing many more details of underlying processes when properly calibrated and validated. They also tend to be more useful forecasting (extrapolation) tools than simpler models, because they tend to include a greater representation of the physics, chemistry, and biology of the physical system being modeled (NRC 2000). A great danger in complex mathematical models is that error propagation is difficult to explicitly measure, and there is a tendency to use a more complex model than required, which drives costs up substantially and unnecessarily. Another consideration that is gaining acceptance is that mathematical models need to be appropriately scaled to

spatial and temporal processes, or they may suffer problems similar to empirical models when one extrapolates the results of scaled experiments to full-sized natural systems. Also, empirical coefficients introduced into equations often hide the degree of uncertainty concerning the fundamental nature of the processes being represented.

Use of Empirical Models in Nutrient Criteria Development

Statistical models are empirical and are derived from observations. To be useful as predictive tools, relationships must have a basis in our understanding, typically represented by conceptual models. However, extrapolation from empirical data is known to be uncertain. Thus, these models are most reliable when used within the range of observations used to construct the model. When shown to meet program objectives and requirements, empirical models are a desirable place to begin model development and, if later determined to be required, they often provide insights into the structure needed for development of mathematical models. Empirical models typically are useful if only a subsystem of the larger ecosystem is of primary interest.

Frequently, the impression is given that the only credible water quality modeling approach is that of mathematical process-based dynamic computer modeling. This is not the case. For example, a Tampa Bay water quality modeling workshop in 1992 (Martin et al. 1996) produced the consensus recommendation that a multipronged (mechanistic and empirical) modeling approach be implemented to provide technical support for the water quality management process. The Tampa Bay National Estuary Program produced an empirical regression-based water quality model. The estimated N loads were related to observed chlorophyll concentrations using the regression model (Janicki and Wade 1996):

$$C_{t,s} = \alpha_{t,s} + \beta_s * L_{t,s}$$

where $C_{t,s}$ = average chlorophyll *a* concentration at month *t* and segment *s*,

$L_{t,s}$ = total N load at month *t* and segment *s*,

$\alpha_{t,s}$ and β_s are regression parameters.

A related model equated Secchi depth to average chlorophyll *a* concentrations (Greening et al. 1997). This analysis was followed by an empirical model that related N loadings to in-bay chlorophyll *a* concentrations.

There are many other examples of empirical models used to relate environmental forcing functions to ecological responses, especially nutrient load/concentration and response relationships. Much of the professional aquatic ecological literature reports on use of empirical models (e.g., Chapters 2 and 3). Empirical models have their limitations, but when judiciously applied, they offer a highly useful tool to water quality managers.

Use of Mathematical Models in Nutrient Criteria Development

Mathematical models can play an important role in assessing acceptable nutrient loads and concentrations in estuaries and near-coastal areas. For example, models are used to:

- Develop a relationship between external nutrient loads and resulting nutrient concentrations, which can then be used to define allowable loads
- Define the relationship between nutrient concentrations and other endpoints of concern, such as biomass or dissolved oxygen
- Provide an increased understanding of the factors affecting nutrient concentrations, such as the relative importance of point and nonpoint source loads
- Simulate relationships between light attenuation and expected depth of sea grass growth

The intent of this section is to describe the models available for assessing the relationship between nutrient loading and nutrient-related water quality criteria for estuaries and near-coastal waters. This chapter provides general guidance and some specific procedures for selecting and applying an appropriate model. It is divided into the following sections: (1) Model Identification and Selection, (2) Model Classification, (3) Use of Models for Nutrient Investigation, and (4) Management Applications.

Extensive EPA guidance (i.e., U.S. EPA 1985, 1990a-c; 1997; EPA document # 841-B-97-006) currently exists on these topics. This section serves primarily to condense the existing guidance with some modifications, to reflect changes in the science that have occurred subsequent to their publication. In addition, emphasis is placed on the simpler, more empirical techniques that are applied most easily. Readers are referred to the original guidance materials for more detailed discussions of the concepts described in this section.

9.2 MODEL IDENTIFICATION AND SELECTION

The first steps in the modeling process are model identification and selection. The goals are to identify the simplest model(s) that addresses all of the important phenomena affecting the water quality problems, and to select from those the most useful analytical formula or computer model. Selection of too simple a model can result in predictions of future water quality that are too uncertain to achieve the decisions or objectives of the study. On the other hand, selection of an overly complex model may also result in misdirected study resources, delays in the study, and increased cost. Predictive uncertainty may increase to unacceptable levels because of model parameters that cannot be adequately estimated with available data. Study costs will increase because of the additional data requirements and the expanded computer and staff time needed for model runs, analysis, and sensitivity studies.

Model Identification

Model identification entails four basic steps:

- Establish study objectives and constraints
- Determine water quality pollutant interactions
- Determine spatial extent and resolution
- Determine temporal extent and resolution

Each is discussed below.

Study Objectives and Constraints

The first step in identifying an appropriate model for a particular site is to clearly delineate the objectives of the modeling analysis. These objectives address questions such as:

- What are the nutrients of concern?
- What are the environmental endpoints of concern?
- What spatial and temporal scales are adequate for management concern?
- What management issues must the model address?
- What is the acceptable level of uncertainty in model predictions?

The nutrients of concern addressed in this document are nitrogen or phosphorus (depending on which is the limiting nutrient or will become limiting after controls are implemented). Environmental endpoints of concern are total nutrient concentration and other indicators of excessive nutrients such as chlorophyll/biomass and minimum dissolved oxygen. Local, State, and Federal regulations contribute to the definition of objectives by specifying time and space scales that the model must address: for example, the averaging period, or the season at which the criteria are applicable.

All expected uses of the model are to be stated clearly in advance. If the model will be used to predict future allowable nutrient loads, the specific conditions to be evaluated must be known. Then a final study objective is established that pertains to the required degree of reliability of model predictions, which may vary depending on whether the model application is designed for screening level estimation or for more detailed predictions.

The reliability objective is directly related to project constraints, as there is often a mismatch between desired model reliability and available resources. Resource constraints can cover four areas: data, time, level of effort, and expertise. Appropriate model selection must be balanced between competing demands. Management objectives typically favor a high degree of model reliability, but resource constraints generally prohibit the degree of reliability desired. Decisions often are required regarding whether to proceed with a higher-than-desired level of uncertainty, or to postpone modeling until additional resources can be obtained.

Water Quality/Pollutant Interactions

After the pollutants and water quality indicators are identified, the significant water quality processes must be determined. These processes directly or indirectly link the pollutants to be controlled with the primary water quality indicators. All other interacting water quality constituents thought to be significant should be included at this point. This consolidation can best be seen in a diagram or flow chart representing the mass transport and transformations of water quality constituents in a defined segment of water. Figure 9-1 illustrates variables and processes important to the eutrophication process. Not all of these need to be included in the actual model selected for use. Those excluded, however, should be considered externally and reflected in the coefficients.

At the end of this step all the available knowledge of a system should be assimilated in a way that permits major water quality processes and ecological relationships to be evaluated for inclusion in the numerical model description. This conceptual model is the starting point from which systematic reductions in complexity can be identified to provide an adequate representation of the system while meeting the objectives of the study.

The simplest level of model complexity considers only total nutrient concentrations and assumes that all of the processes shown in Figure 9-1 either have no effect on total nutrient concentrations (as is sometimes assumed for total nitrogen), or can be lumped into a single overall loss coefficient.

Models that simulate phytoplankton concentrations or dissolved oxygen typically include all of the processes shown in Figure 9-1, and sometimes many more, to describe such processes as sediment diagenesis and competition among multiple phytoplankton classes. Denitrification in the model is expressed in terms of the water column carbonaceous biochemical oxygen demand (CBOD).

Spatial Extent and Scale

Two spatial considerations must be addressed in the model identification process: spatial extent and scale. Spatial extent pertains to the specific boundaries of the area to be assessed. Spatial scale pertains to the number of dimensions to be considered and the degree of resolution to be provided in each dimension.

Several guidelines can help locate proper model boundaries. In general, the boundaries should be located beyond the influence of the discharge(s) being evaluated. Otherwise, proper specification of boundary concentrations for model projections is very difficult. Boundaries should be located where flow or stage and water quality are well monitored. Upstream boundaries should be located at a fall line, or at a gaging station in free-flowing, riverine reaches. Downstream boundaries are best located at the mouth of an estuary, or even nearby in the ocean. For large estuaries with relatively unaffected seaward reaches, the downstream boundary can be located within the estuary near a tidal gage and water quality monitoring station.

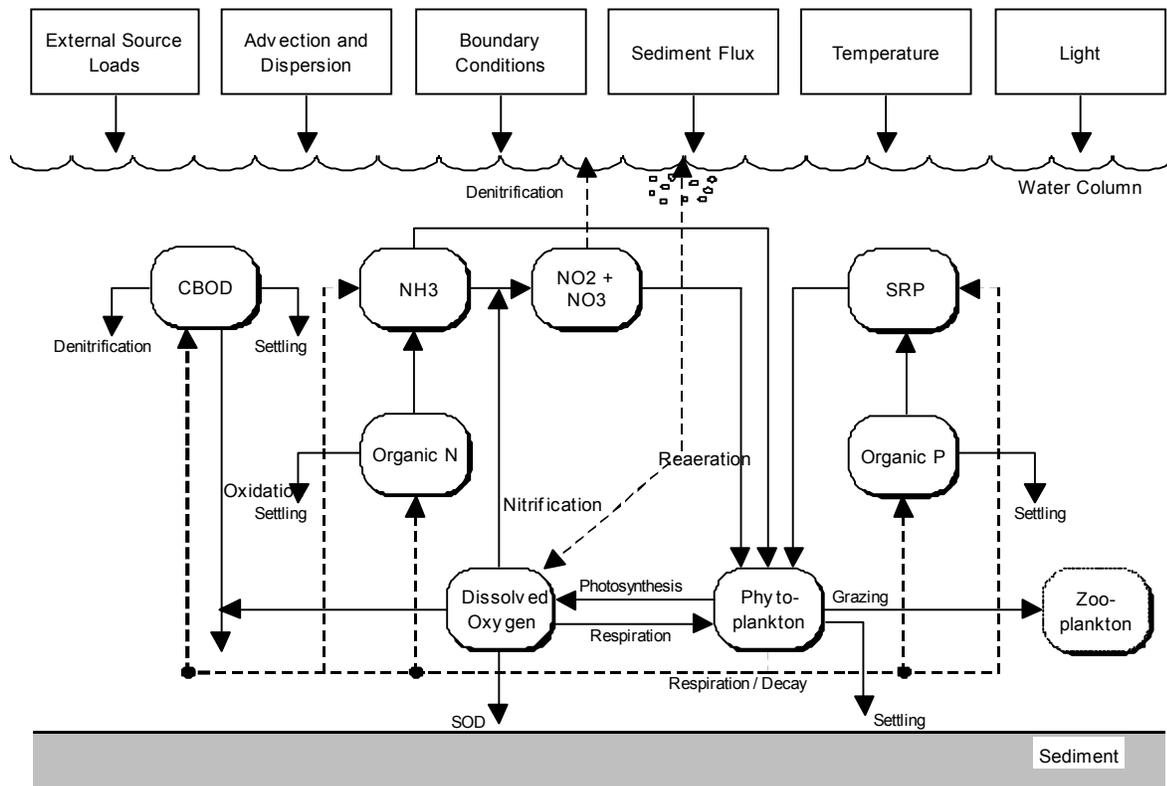


Figure 9-1. Eutrophication model framework : an example of hypoxia-based conceptual framework for water quality model. Source: Bierman et al. 1994.

Appropriate model spatial scale requires consideration of two factors: (1) the extent to which spatial gradients in water quality occur and (2) the extent to which these variations need to be considered from a management perspective. Real estuaries and near-shore waters all exhibit three-dimensional properties. There are gradients in hydrodynamic and water quality constituents over length, width, and depth. The effective dimensionality of an estuary includes only those gradients that affect the water quality analysis significantly.

One-dimensional models consider the change in pollutant concentration over a single dimension in space, typically oriented longitudinally down the length of an estuary. Two-dimensional models can consider concentration gradients in the lateral and longitudinal directions (termed x-y orientation), or concentration gradients that occur longitudinally and vertically (termed x-z orientation). Three-dimensional models describe changes in concentration that occur over all three spatial dimensions. These models provide the most detailed assessment of pollutant distribution with respect to a discharge; they also have the most extensive model input requirements and are the most difficult to apply.

Justifiable reductions in dimensionality result in savings in model development, simulation, and analysis costs. Usually the vertical and/or lateral dimension is neglected. Eliminating a dimension from the water quality analysis implies acceptable uniformity of water quality constituents in that spatial dimension. For example, use of one-dimensional models implies acceptably small deviations in concentration from the

cross-sectional mean, both vertically and laterally. This judgment requires understanding both the transport behavior of estuaries and the specific objectives of the study.

Spatial variations are best determined by plotting observed water quality concentrations versus distance along the dimensions of concern. If such data are not available, other types of methods are available to estimate the importance of spatial variations. These are described in U.S. EPA (1990a) and discussed briefly here. The methods can be divided into three categories:

- Relatively simple desktop methods that compare the stratification potential caused by freshwater inputs to the mixing potential caused by tides and other currents
- Dye studies that observe the degree of mixing
- Geomorphological classification, which categorizes estuaries and the degree of mixing based on standard morphological categories (e.g., drowned river valleys)

Two situations exist where the observed spatial variations can be ignored. The first is when the primary location of water quality concern occurs in an area where these gradients are not important. A good example would be a nutrient modeling study to consider the impacts of a discharge on phytoplankton. If it takes 2 miles for a bankside discharge to undergo complete lateral mixing, but the location of maximum algal density is 5 miles downstream, lateral variability in water quality need not be described by the model. The second situation where a known gradient need not be modeled is where management objectives are not concerned with the gradient. Examples of this include water quality standards that are expressed on a spatially averaged basis.

The choice of spatial scale and layout of the model network requires considerable judgment. Knowledge of the regulatory problem must be combined with knowledge of the loading, transport, and transformation processes and an understanding of the model chosen to perform the simulations. Competing factors often must be balanced, such as precision and cost, or the better fit of one section of the network versus another.

Temporal Extent and Scale

The temporal resolution of water quality models falls into one of two broad categories, steady state or dynamic (i.e., time-variable). Steady-state models predict pollutant concentrations that are expected to result from a single set of loading and environmental conditions. Dynamic models predict changes in water quality over time in response to time-variable loads and environmental conditions.

Steady-state models are much easier to apply and require considerably fewer resources than dynamic models. This ease of application makes them the preferred modeling framework when loading to the system can be assumed to be constant and information on changes in concentration over time is not required. Potential uses of steady-state models include calculation of seasonal average total nutrient concentrations in response to seasonal average loads. Steady-state models also have been used to predict

“critical condition” low-flow phytoplankton densities. Steady-state models are poorly suited for evaluating individual intermittent events (i.e., runoff) but can be used to evaluate the cumulative effect of multiple, intermittent events on a seasonal basis.

The timeframe to be represented for a particular steady-state simulation (e.g., monthly average, seasonal average) must be longer than the water residence time (flushing time) of the estuary. The water residence time is the time required to remove a parcel of water from an upstream location in an estuary. Factors that control flushing include tidal action, freshwater inflow, and wind stress. Typical flushing times range from days in small estuaries, or those dominated by tributary flow, to months in large estuaries during low tributary flow conditions. Several formulae have been used to estimate flushing times. The Fraction of Fresh Water Method, the Tidal Prism Method, and the Modified Tidal Prism Method are fully discussed in Mills et al. (1985) and briefly described in the following section.

Dynamic models should be used when information on changes in concentration over time is required. Dynamic models can be divided into two categories, quasi-dynamic and fully dynamic. Quasi-dynamic simulations predict variations on the order of days to months. The effects of tidal transport are time-averaged, and net or residual flows are used. Fully dynamic simulations predict hour-to-hour variations caused by tidal transport.

The duration of dynamic simulations can range from days to years, depending on the size and transport characteristics of the study area, the reaction kinetics and forcing functions of the water quality constituents, and the strategy for relating simulation results to the regulatory requirements. One basic guideline applies in all cases: the simulations should be long enough to eliminate the effect of initial conditions on important water quality constituents at critical locations. Flushing times provide the minimum duration for simulations of dissolved, nonreactive pollutants. The annual sunlight and temperature cycles almost always require that eutrophication simulations range from seasons to years.

Predicting the year-to-year eutrophication response of large estuaries is best accomplished by quasi-dynamic simulations. In general, if the regulatory need or kinetic response is on the order of hours, then fully dynamic simulations are required; if regulatory needs are long-term averages and the kinetic response is on the order of seasons to years, then quasi-dynamic or steady-state simulations are preferred.

Model Selection

The goal of model selection is to obtain a simulation model that effectively meets all study objectives. In the final analysis, how a model is used is more important to its success than exactly which model is used. Nevertheless, although selection of an appropriate model will not guarantee success, it will help. Selection of an inappropriate model will not guarantee failure, but will render a successful outcome more difficult.

Models may be classified in different and somewhat arbitrary ways. Some models may not quite fit in any category, or may fit well in several. In addition, models tend to evolve with use. The exact capabilities of the individual models described here may change. In particular, pollutant fate processes

may be modified. Usually the computational framework and the basic transport scheme remain stable over time. For this reason, transport characteristics will provide the basis for the model classification scheme used here. Models selected for discussion here are general purpose, in the public domain, and available from or supported by public agencies.

9.3 MODEL CLASSIFICATION

Estuarine and near-coastal models consist of two components: hydrodynamics and water quality. Although the hydrodynamic component is independent of the water quality component, water quality depends on the transport processes controlled by hydrodynamics. As a result, estuarine models can be classified as Level I to Level IV, according to the temporal and spatial complexity of the hydrodynamic component of the model.

Level I includes desktop screening methodologies that calculate seasonal or annual mean total nutrient concentrations based on steady-state conditions and simplified flushing time estimates. Steady-state models use an unvarying flow condition that neglects the temporal variability of tidal heights and currents. These models are designed for relatively simple screening level analyses. They also can be used to highlight major water quality issues and important data gaps in the early model-identification stage of a more complex study.

Level II includes computerized steady-state or tidally averaged quasi-dynamic simulation models, which generally use a box or compartment-type network. Tidally averaged models simulate the net flow over a tidal cycle. These models cannot predict the variability and range of nutrient concentrations throughout each tidal cycle, but they are capable of simulating variations in tidally averaged concentrations over time. Level II models can predict slowly changing seasonal water quality with an effective time resolution of 2 weeks to 1 month.

Level III includes computerized one-dimensional (1-d) and quasi two-dimensional (2-d) dynamic simulation models. These real-time models simulate variations in tidal heights and velocities throughout each tidal cycle. One-dimensional models treat the estuary as well-mixed vertically and laterally. Quasi 2-d models employ a link-node approach that describes water quality in two dimensions (longitudinal and lateral) through a network of 1-d nodes and channels. Tidal movement is simulated with a separate hydrodynamic package in these models. The required data and modeling resources typically are unavailable to support models of Level III or above on a widespread basis.

Level IV consists of computerized 2-d and 3-d dynamic simulation models. Dispersive mixing and seaward boundary exchanges are treated more realistically than in the Level III 1-d models. These models are almost never used for routine nutrient assessment, because of excessive resource requirements.

Level I Models

Level I desktop methodologies may be employed using a hand-held calculator or computer spreadsheet and are based on steady-state conditions, first-order decay coefficients, simplified estimates of flushing time, and seasonal pollutant concentrations. The EPA screening methods provide a series of Level I analyses as described below.

EPA Screening Methods

WQAM is a set of steady-state desktop models that includes both one-dimensional and two-dimensional box model calculations (Mills et al. 1985). Specific techniques contained in WQAM are the Fraction of Freshwater Method, the Modified Tidal Prism Method, Advection-Dispersion Equations, and Pritchard's Two-Dimensional Box Model.

Fraction of Freshwater Method

The Fraction of Freshwater Method estimates pollutant concentrations in one-dimensional estuaries from information on freshwater and tidal flow by comparing salinity in the estuary with salinity in the local seawater. The fraction of freshwater at any location in the estuary is calculated by comparing the volume of freshwater at that location with the total volume of water:

$$f_x = \frac{S_s - S_x}{S_s} \quad (9-1)$$

where f_x = fraction of freshwater at location x , S_s = seawater salinity at the mouth of the estuary, and S_x = salinity at location x .

This ratio can be viewed as the degree of dilution of the freshwater inflow (as well as pollutants) by seawater. With this in mind, the total dilution of a pollutant input can be calculated by multiplying the seawater dilution by the freshwater dilution. This then provides a simple way to calculate concentrations of conservative pollutants. For any location x , at or downstream of the discharge, pollutant loads are diluted by tidal mixing and upstream flows. The amount of dilution can be calculated by:

$$C_x = f_x \frac{W}{Q} \quad (9-2)$$

where C_x = constituent concentration at location x at or downstream of discharge, f_x = fraction of freshwater at location x , W = waste loading rate (mass/time), and Q = freshwater inflow (volume/time).

The right side of Equation 9-2 can be divided into two distinct terms. The term W/Q represents the classical equation for determining dilution in rivers caused by upstream flow. The second term, f_x , accounts for the further dilution of the river concentration by tidal influx of seawater.

Concentrations upstream of the discharge are estimated from the concentration at the point of mix and the relative salinity of the upstream location. The upstream concentrations are assumed to be diluted by freshwater to the same degree that salinity is diluted. The equation is:

$$C_x = f_d \frac{W}{Q} \frac{S_x}{S_d} \quad (9-3)$$

where f_d = fraction of freshwater at discharge location, S_x = salinity at upstream location x , and S_d = salinity at discharge location.

The fraction of freshwater at the discharge location, f_d , is determined by applying Equation 9-1 at the discharge location. Equation 9-3 can be modified to assess the impact of nutrients entering from the seaward boundary by replacing the leading $f_d W/Q$ term with the boundary nutrient concentration.

Cumulative pollutant impacts from multiple sources are obtained through a two-step process. First, pollutant concentration caused by each source independent of all other discharges must be determined. This determination is accomplished by applying Equation 9-2 or 9-3, one discharge at a time, for any estuary location of interest. The second step is to determine the total concentration at that location. This determination is accomplished by adding all of the incremental concentrations caused by each discharge, as calculated in the first step. This process can be repeated for any location of interest.

The Fraction of Freshwater Method can be used to predict cumulative impacts in one-dimensional (i.e., narrow) systems with significant freshwater inflow. Upstream freshwater flow must be large with respect to total pollutant inflow for this method to be applicable. The method assumes conservative pollutant behavior. It is consequently best used to investigate total nitrogen concentrations, because overall loss rates of total nitrogen from the water column generally are small.

Modified Tidal Prism Method

The Modified Tidal Prism Method estimates dilution from the total amount of water entering an estuary. It is more powerful than the Fraction of Freshwater Method because it can consider not only tidal dilution but also nonconservative reaction losses. It is best applied to investigate total nutrient concentrations, but provides additional flexibility to describe pollutant losses that may occur through settling or denitrification.

The method divides an estuary into segments whose lengths and volumes are calculated using low-tide volumes and tidal inflow. The tidal prism (i.e., total volume of tidal inflow) is compared for each segment with the total segment volume to estimate flushing potential in that segment over a tidal cycle. The Modified Tidal Prism Method assumes complete mixing of the incoming tidal flow with the water resident in each segment.

The Modified Tidal Prism Method requires seven inputs:

- Freshwater inflow to the estuary
- Salinity of seawater at the downstream boundary
- Pollutant loading rate
- Salinity of each segment
- Low-tide volume for each segment
- Intertidal volume (tidal prism) for each segment
- First-order constituent loss rate for each segment

The first step of the method is to segment the estuary. This requires an initial time-consuming step of dividing the estuary into segments with lengths equal to the distance traveled by a particle over a tidal cycle. Cumulative subtidal and intertidal water volumes must be plotted for the estuary, and a graphical procedure is used to define model segmentation. Once the estuary has been segmented, a series of calculations can be performed to estimate constituent concentrations in each segment. Specific methods for dividing the estuary and performing the calculations are provided in Mills et al. (1985).

Advection-Dispersion Equations

Analytical equations have been developed to predict the concentration of nonconservative constituents in one-dimensional estuaries. These types of equations consider the processes of net seaward flows (advection) and tidally averaged mixing (dispersion), as well as simple decay. They can be used to predict total nutrient concentrations at various locations in an estuary in response to alternative nutrient loading rates. One-dimensional advection-dispersion equations can be expressed in several different forms (O'Connor 1965), with the most common form contained in the water quality assessment methodology. These equations require numerous simplifying assumptions, such as constant geometry and tidal mixing along the length of the estuary, but have proven to be a useful screening tool.

The advection-dispersion equations require five inputs: upstream freshwater flow rate (R), constituent loading rate (W), estuarine cross-sectional area (A), tidally averaged dispersion coefficient (E), and first-order decay rate coefficient (k). The first three inputs can be measured directly. The latter two inputs must be determined indirectly through the model calibration process described below. Two equations are provided, one which predicts concentrations at any distance (x) upstream of the discharge of concern and another for concentrations at any distance seaward of the discharge. C_0 is the concentration at the point of discharge. The equations are:

$$C = C_0 e^{j_2 x} \quad X > 0 \text{ (down estuary)} \quad (9-4)$$

$$C = C_0 e^{j_1 x} \quad X < 0 \text{ (up estuary)}$$

where:

$$j_2 = \frac{R}{2AE} \left(1 - \sqrt{1 + \frac{4kEA^2}{R^2}} \right)$$

$$j_1 = \frac{R}{2AE} \left(1 + \sqrt{1 + \frac{4kEA^2}{R^2}} \right)$$

$$C_0 = \frac{W}{R} \frac{1}{\sqrt{1 + (4kE / U^2)}}$$

These equations can be used to evaluate multiple loading sources by independently applying Equation 9-4 for each loading source and summing the predicted concentrations across the estuary.

Pritchard's Two-Dimensional Box Model

Vertically stratified estuaries add a significant degree of complexity to the modeling analysis. Pritchard (1969) developed a relatively simple approach, which can predict nutrient concentration distributions along the length of an estuary in both an upper and lower layer. This approach is based on numerous simplifying assumptions, including:

- Steady-state conditions
- Conservative pollutant behavior
- Uniform constituent concentration within each layer or each segment

The following information is required: (1) freshwater flow rate into the head of the estuary, (2) pollutant mass loading rates, and (3) longitudinal salinity profiles along the length of the estuary in the upper and lower layers. The method solves a series of linear equations describing the salinity balance around each segment to determine net flows and dispersion between each segment. Specific methods for performing the calculations are provided in Mills et al. (1985).

Results from Pritchard's model can be used to directly calculate conservative constituent concentrations throughout the estuary or to serve as the hydrodynamic input to one of the Level II models described below.

Level II Models

Level II models include computerized steady-state and tidally averaged simulation models that generally use a box or compartment-type network. Steady-state models are difficult to calibrate in situations where hydrodynamics and pollutant releases vary rapidly. Consequently, these models are less appropriate when waste load, river inflow, or tidal range vary appreciably with a period close to the flushing time of the waterbody. Level II models are the simplest models available that are capable of describing the

relationship between nutrient loads and some of the endpoints of concern of the eutrophication process (i.e., chlorophyll *a*, minimum dissolved oxygen).

The Level II models by EPA are QUAL2E and the Water Quality Analysis Simulation Program (WASP5), with its associated eutrophication program EUTRO5.

QUAL2E

QUAL2E is a steady-state, one-dimensional model designed for simulating conventional pollutants in streams and well-mixed lakes (U.S. EPA 1995) and is not recommended for estuaries. Rather, QUAL TX, which allows tidal boundary conditions, may be more appropriate, but documentation on this model is very sparse.

WASP6.0

The Water Quality Analysis Simulation Program (WASP6.0) is a general, multidimensional model that utilizes compartment modeling techniques (Ambrose et al. 1993). The equations solved by WASP6.0 are based on the principle of conservation of mass. Operated in the quasi-dynamic mode, WASP6.0 requires the user to supply initial segment volumes, network flow fields, and inflow time functions. The user also must calibrate dispersion coefficients between compartments. WASP6.0 has the capability of simulating nutrient-related water quality issues at a wide range of complexity.

EUTRO5

EUTRO5 is the submodel in the WASP6.0 system that is designed to simulate conventional pollutants. EUTRO5 combines a kinetic structure adapted from the Potomac Eutrophication Model with the WASP transport structure. EUTRO5 predicts DO, carbonaceous BOD, phytoplankton carbon and chlorophyll *a*, ammonia, nitrate, organic nitrogen, organic phosphorus, and orthophosphate in the water column and, if specified, the underlying bed. In addition to segment volumes, flows, and dispersive exchanges, the user must supply deposition and resuspension velocities for organic solids, inorganic solids, and phytoplankton. Rate constants and half-saturation coefficients for the various biochemical transformation reactions must be specified by the user. Finally, the time- and/or space-variable environmental forcing functions, such as light intensity, light extinction, wind speed, cloud cover, temperature, and benthic fluxes, must be input.

Level III Models

Level III includes computerized 1-d and 2-d models that simulate variations in tidal height and velocity throughout each tidal cycle. Level III models enable characterization of phenomena varying rapidly within each tidal cycle, such as pollutant spills, stormwater runoff, and batch discharges. Level III models also are deemed appropriate for systems where the tidal boundary impact, as a function of the hydrodynamics and water quality, is important to the modeled system within a tidal period.

Tidally varying (intratidal) models have found most use in the analysis of short-term events, in which the model simulates a period of time anywhere from one tidal cycle to a month. Some seasonal simulations also have been conducted.

In using Level III models, one must decide whether a 1-d longitudinal system is sufficient, or whether a 2-d model is required to capture the longitudinal and lateral variations in the estuary. For estuaries whose channels are longer than their width and reasonably well mixed across their width, a 1-d model may be chosen. If large differences exist in water quality from one side of an estuary to the other, or if vertical stratification is important, then a 2-d model is appropriate.

All Level III models considered here can simulate nutrient-eutrophication interactions. These models also include settling rates and benthic flux rates for several different constituents, such as phosphorus, nitrogen, and sediment oxygen demand. The Level III model distributed by EPA is the WASP6.

Level IV Models

Level IV includes a variety of computerized 2-d and 3-d dynamic simulation models. Dispersive mixing and seaward boundary exchanges are treated more realistically than in the Level III 1-d models. Although not routinely used in nutrient analyses, they are now finding use by experts in special studies. Level IV models are required when variations in concentrations in all three dimensions are of concern. The time-variable nature of a Level IV model ensures the need for a time-variable watershed model in order to provide for the nonpoint source inputs. Fully 3-d models that can predict longitudinal, lateral, and vertical transport are the most complex and expensive to set up and run.

At present, no Level IV model is supported by EPA. Three current Level IV models, CE-QUAL-W2, Integrated Compartment Model (ICM), and EFDC, are described below.

CE-QUAL-W2

CE-QUAL-W2 is a dynamic 2-d (x-z) model developed for stratified waterbodies (Environmental and Hydraulics Laboratories 1986). This is a U.S. Army Corps of Engineers modification of the Laterally Averaged Reservoir Model (Edinger and Buchak 1983; Buchak and Edinger 1984a,b). CE-QUAL-W2 consists of directly coupled hydrodynamic and water quality transport models. Hydrodynamic computations are influenced by variable water density caused by temperature, salinity, and dissolved and suspended solids. Developed for reservoirs and narrow, stratified estuaries, CE-QUAL-W2 can handle a branched and/or looped system with flow and/or head boundary conditions. With two dimensions depicted, point and nonpoint loadings can be distributed spatially.

CE-QUAL-W2 simulates as many as 20 other quality variables. Primary physical processes included are surface heat transfer, shortwave and longwave radiation and penetration, convective mixing, wind- and flow-induced mixing, entrainment of ambient water by pumped-storage inflows, inflow density current placement, selective withdrawal, and density stratification as influenced by temperature and dissolved and suspended solids. Major chemical and biological processes in CE-QUAL-W2 include the effects on DO of atmospheric exchange, photosynthesis, respiration, organic matter decomposition, nitrification, and chemical oxidation of reduced substances; uptake, excretion, and regeneration of phosphorus and nitrogen and nitrification-denitrification under aerobic and anaerobic conditions; carbon cycling and alkalinity-pH-CO₂ interactions; trophic relationships for total phytoplankton; accumulation and decomposition of detritus and organic sediment; and coliform bacteria mortality.

CH3D-ICM

CH3D is a 3-d, finite-difference hydrodynamic model, developed by the U.S. Army Corps of Engineers Waterways Experiment Station (WES) in Vicksburg, MS. Results from CH3D have been linked to the ICM to model water quality in the Chesapeake Bay. The ICM was developed as the integrated-compartment eutrophication model component of the Chesapeake Bay model package. The model contains detailed eutrophication kinetics, modeling the carbon, nitrogen, phosphorus, silica, and dissolved oxygen cycles.

CH3D-ICM is a linkage of CH3D, a hydrodynamic model, and ICM, a water quality model. CH3D is a hydrodynamic model developed for the Chesapeake Bay Program (Johnson et al. 1991). The model can be used to predict system response to water levels, flow velocities, salinities, temperatures, and the three-dimensional velocity field. CH3D makes hydrodynamic computations on a curvilinear or boundary-fitted platform grid. Deep navigation channels and irregular shorelines can be modeled because of the boundary-fitted coordinates feature. Vertical turbulence is predicted by the model and is crucial to a successful simulation of stratification, destratification, and anoxia. A second-order model based on the assumption of local equilibrium of turbulence is employed.

ICM is a finite-difference water quality model that may be applied to most waterbodies in one, two, or three dimensions (Cercio and Cole 1995). The model predicts time-varying concentrations of water quality constituents and includes advective and dispersive transport. The model also considers sediment diagenesis benthic exchange. ICM incorporates detailed algorithms for water quality kinetics. Interactions among state variables are described in 80 partial-differential equations that employ more than 140 parameters. An improved finite-difference method is used to solve the mass conservation equation for each cell in the computational grid and for each state variable.

EFDC

EFDC is a linked three-dimensional, finite-difference hydrodynamic and water quality model developed at the Virginia Institute of Marine Sciences (Hamrick 1996). EFDC contains extensive water quality capabilities, including a eutrophication framework based on the ICM model. EFDC is a general-purpose hydrodynamic and transport model that simulates tidal, density, and wind-driven flow; salinity; temperature; and sediment transport. Two built-in, full-coupled water quality/eutrophication submodels are included in the code.

EFDC solves the vertically hydrostatic, free-surface, variable-density, turbulent-averaged equations of motion and transport; transport equations for turbulence intensity and length scale, salinity, and temperature in a stretched, vertical coordinate system; and horizontal coordinate systems that may be Cartesian or curvilinear-orthogonal. Equations describing the transport of suspended sediment, toxic contaminants, and water quality state variables also are solved.

The model uses a finite-difference scheme with three time levels and an internal-external mode splitting procedure to achieve separation of the internal shear, or baroclinic, mode from the external free-surface gravity wave, or barotropic, mode. An implicit external-mode solution is used with simultaneous

computation of a two-dimensional surface elevation field by a multicolor successive overrelaxation procedure. The external solution is completed by calculation of the depth-integrated barotropic velocities using the new surface elevation field. Various options can be used for advective transport, including the “centered in time and space” scheme and the “forward in time and upwind in space” scheme.

Summary of Model Capabilities

The important features of the models selected for discussion in this manual are summarized in Tables 9-1 and 9-2. The information provided in these tables is primarily qualitative and sufficient to determine whether a model may be suitable for a particular application. For complete information, consult the appropriate user's manuals, the supporting agency, and other experienced users.

9.4 USE OF MODELS FOR NUTRIENT INVESTIGATION

This section describes procedures for using models to perform nutrient assessment in estuaries and near-coastal waters. It describes the model calibration and validation process, where model parameters that best describe the waterbody of interest are selected. In addition, guidance is provided on using models for nutrient management and assessment.

The first subsection describes a general procedure for calibrating nutrient models, and briefly describes the validation procedure used to estimate the uncertainty of such models. The subsection also describes some statistical methods for testing the calibrated models. These methods are useful to aid in the various calibration phases and also in the validation phase to measure how well model predictions and measurements of water quality agree.

The second subsection provides guidance on the management application of a calibrated model. Methods to project effects of changes in waste loads and to determine causes of existing conditions are discussed. Finally, a case study application is provided.

Model Calibration and Validation

Model calibration is the process of determining model parameters most appropriate for a given site-specific application. Calibration of a model involves a comparison of the measured and simulated receiving water quality conditions. The nature of the model calibration process depends upon the complexity of the model selected. Simpler models contain relatively few parameters that need to be calibrated, whereas more complex models contain many.

Calibration alone is not adequate to determine the predictive capability of a model for a particular estuary. To map out the range of conditions over which the model can be used, one or more additional independent sets of data are required to determine whether the model is predictively valid. This model validation exercise defines the limits of usefulness of the calibrated model. Without validation testing, the model merely describes the conditions defined by the calibration data set. The degree of uncertainty of any projection or extrapolation of the model remains unknown.

Table 9-1. Basic model features

Methods/Model	Time Scales	Spatial Dimensions	Hydro-dynamics	Data Expertise Requirements	Distributing Agency	Scale of Effort
Fraction of Freshwater	SS	1D	0	Minimal	EPA	Days
Modified Tidal Prism	SS	1D	0	Minimal	EPA	Days
Advection-Dispersion Equations	SS	1D	0	Minimal	EPA	Days
Pritchard's 2-D Box Model	SS	2D (xz)	0	Minimal	EPA	Days
QUAL2E	SS	1D	I	Moderate	EPA	Few months
WASP5	Q/D	1D, 2D (xy), or 3D	I, S	Moderate to substantial	EPA	Few months
CE-QUAL-W2	D	2D (xz)	S	Substantial	Army Corps	Several months
CH3D-ICM	D	3D	S	Extreme	EPA	Months to years
EFDC	D	3D	S	Extreme	EPA	Months to years

D - dynamic; Q - quasi-dynamic (tidal-averaged); SS - steady state; x - 1-dimensional, xy - 2-dimensional, longitudinal-lateral; xz - 2-dimensional, longitudinal-vertical; xyz - 3-dimensional; B - compartment or box 3d; xx - link node branching 2d; 0 - No hydraulics specified, inferred from salinity data; I - hydrodynamics input; S - hydrodynamics simulated.

In general, models are calibrated in phases, beginning with the selection of the model parameters and coefficients that are independent of parameters to be calibrated later. For purposes of this discussion, the process is divided into the categories of hydrodynamic calibration and water quality calibration. The discussion covers the parameters that need to be calibrated for each level of model as well as the specific model outputs to be used for the calibration comparison. Calibration of the more complex models requires detailed guidance; the reader is referred to other documents (e.g., U.S. EPA 1990b; Thomann and Mueller 1987) for a discussion that is more comprehensive than is feasible here.

Hydrodynamic Calibration

The first phase of calibration concentrates on the hydrodynamic and mass transport models. Two Level I models, the Fraction of Freshwater Method and the Tidal Prism Method, have no hydrodynamic parameters that require calibration. In these simplest cases, all hydrodynamic and mass transport processes are implicitly considered via specification of observed salinity values. Although there are no parameters to calibrate for these models, there is merit in testing the model's predictive validity by comparing predicted concentrations with field observations of a conservative (i.e., nondecaying) substance, if such data are available.

For the remaining Level I and Level II models, only one hydrodynamic parameter requires calibration: the tidal dispersion coefficient. It is possible to calibrate the hydrodynamic and mass transport portions of these models by determining values for this coefficient that best describe observed salinity or conservative tracer measurements.

Table 9-2. Key features of selected models

Model	Key Features	Advantages	Disadvantages/ Limitations
WQAM	Simplified equations to simulate dilution, advection, dispersion, first-order decay, empirical relationships between nutrient loading, and total nutrient concentration	Few data requirements; can be employed easily with a hand calculator or computer spreadsheet	Limited to screening and midlevel applications
QUAL2E	Steady-state model provides adequate simulation of water quality processes, including DO-BOD and algal growth cycles	User-friendly Windows interface; widely used and accepted; able to simulate all of the conventional pollutants of concern	Limited to simulation of time periods during which stream flow and input loads are essentially constant
WASP5	Based on flexible compartment modeling approach; can be applied in 1, 2, or 3 dimensions	Has been widely applied to estuarine situations; considers comprehensive DO and algal processes; can be used in 3-d simulations by linking with hydrodynamic models	Coupling with multi-dimensional hydrodynamic models requires extensive site-specific linkage efforts
CE-QUAL-W2	Uses an implicit approach to solve equations of continuity and momentum; simulates variations in water quality in the longitudinal and lateral directions	Simulates the onset and breakdown of vertical stratification; most appropriate where vertical variations are an important water quality consideration	Application requires extensive modeling experience
CH3D-ICM	Finite-difference model can be applied to most water bodies in 1 to 3 dimensions; predicts time-varying concentrations of constituents; includes advective and dispersive transport	State-of-the-science eutrophication kinetics	Computationally intensive; requires extensive data for calibration and verification; requires a high level of technical expertise to apply effectively
EFDC	Linked 3-d, finite-difference hydrodynamic and water quality model contains extensive water quality capabilities; water quality concentrations can be predicted in a variety of formats suitable for analysis and plotting	3-d description of water quality parameters of concern; entire range of hydrodynamic, sediment, eutrophication, and toxic chemical constituents can be considered	Computationally intensive; requires extensive data for calibration and verification; requires a high level of technical expertise to apply effectively

Level III models typically contain two calibration parameters, the channel roughness coefficient and the dispersion coefficient. Occasionally these models are calibrated with current velocity and water surface elevation data, but more often are indirectly calibrated from salinity or conservative tracer measurements that also must be used to calibrate the mass transport model. Indirect calibration can result in an imprecise description of both the circulation and mass transport algorithms, but this is not a severe drawback unless the critical water quality components of the waste load allocation model are sensitive to small changes in circulation and mass transport.

Level IV hydrodynamic models contain several calibration parameters, including bottom and surface friction coefficients; vertical, lateral, and horizontal eddy viscosity coefficients; and wind speed coefficients. Calibration efforts for these types of models are beyond the scope of this document.

Kinetic Process Calibration

The second phase of calibration involves selection of the set of kinetic coefficients describing nutrient cycles and other aspects of the eutrophication process. Again, the effort required is directly related to the complexity of the model selected.

Two Level I models—the Fraction of Freshwater Method and Pritchard’s model—have no kinetic parameters that require calibration. The models assume that constituent concentrations undergo no kinetic processes that affect their concentration, and typically are appropriate only for estimating total nitrogen concentrations. The remaining Level I models can describe nonconservative constituents, and lump all kinetic processes into a single overall decay coefficient. Model calibration in these cases consists of a comparison of predicted versus observed total nutrient concentrations.

The calibration of higher level nutrient and phytoplankton models requires significant expertise because of the complexity of the interactions between a number of the components of the cycles involved.

Coefficients that require calibration in these models pertain to: transformation rates among various forms of a given nutrient; maximum phytoplankton growth rates; phytoplankton respiration rates; phytoplankton growth sensitivity to light and nutrients; and phytoplankton and detrital settling velocities.

Model Validation

Validation testing is designed to confirm that the calibrated model is useful at least over the limited range of conditions defined by the calibration and validation data sets. The procedure is not designed to validate a model as generally being useful in every estuary, or even as useful over an extensive range of conditions found in a single estuary. Validation, as employed here, is limited strictly to indicating that the calibrated model is capable of producing valid results over a limited range of conditions. Those conditions are defined by the sets of data used to calibrate and validate the model. As a result, it is important that the calibration and validation data cover the range of conditions over which predictions are desired.

Validation testing is performed with an independent data set collected during a second field study. The field study may occur before or after the collection of calibration data. For the best results, however, the validation data should be collected after the model has been calibrated. This schedule of calibration and validation ensures that the calibration parameters are fully independent of the validation data. Often it is difficult to assemble the necessary resources to conduct the desired number of surveys. Therefore, it is important that surveys be scheduled in an innovative manner and the choice of calibration and validation data sets remain flexible to make the test of the calibrated model as severe as possible.

Too often, limited studies attempt calibration but not validation. This approach, in effect, limits the study to describing the conditions during the calibration data collection period and increases the uncertainty associated with the waste load allocation. In fact, model prediction uncertainty cannot be reliably assessed in these cases.

Model Testing

During and after the calibration and validation of a model, at least two types of testing are important. First, throughout the calibration procedure, a sensitivity test helps determine which parameters and coefficients are the most important. Second, a number of statistical tests help define the extent of agreement between model simulations and measured conditions.

The sensitivity analysis is simply an investigation of how much influence changes in model coefficients have on simulated results. Typically, important coefficients, parameters, boundary conditions, and initial conditions are varied by a positive or negative constant percentage to see what effect the change has on critical predictions. The coefficients and parameters are changed one at a time and the effects typically are ranked to show which parameters have the most influence and which have the least.

The second type of testing involves assessment of the “goodness of fit” for model simulations, compared with measurement of important water quality parameters. In addition to making a visual assessment, a number of statistical tests have proven useful. These include root mean square error, relative error, and regression analysis. Other more detailed statistical analyses are described in U.S. EPA (1990b). The root mean square (rms) error is a criterion that is widely used to evaluate the agreement between model predictions. The rms error can be defined as:

$$rms = \left[\sum (C_m - C_s)^2 N \right]^{0.5} \quad (9-5)$$

where C_m = measured concentration, C_s = simulated concentration, and N = number of measurements.

The rms error can be used to compute simultaneous discrepancies at a number of points, or it can be used to compute discrepancies between measurements and predictions at a single point over time. Global rms errors can be computed for a series of measurements at multiple points over time.

When discrepancies between model simulations and measurements are not uniform over parts of the estuary or over time, the relative error may be a more appropriate statistic for testing calibration or validation. The relative error is defined as:

$$e = \frac{|\overline{C}_m - \overline{C}_s|}{\overline{C}_m} \quad (9-6)$$

where the overbars denote the average measured or simulated value. Averages can be performed over multiple sites or over time. The relative error behaves poorly for small values of measurements if discrepancies are not proportional to the magnitude of the measurement (i.e., small values of C_m magnify discrepancies) and if $C_m > C_s$ (as the maximum relative error is usually taken to be 100%). Therefore, the relative error is best for computing composite statistics when discrepancies are not constant, as may occur when calibration over an extensive range is attempted.

Regression analysis is very useful in identifying various types of bias in predictions of dynamic-state variables. The regression equation is written as:

$$C_m = a + bC_s + \epsilon \quad (9-7)$$

where a = intercept value, b = slope of the regression line, and ϵ = the error in measurement mean, C_m . The standard linear regression statistics computed from the above equation provide insight into the goodness of fit for a calibration. The square of the correlation coefficient, r^2 , measures the percent of the variance accounted for between measured and predicted values. The slope estimate, b , and intercept, a , can indicate any consistent biases in the model calibration. A model calibration that perfectly described all available data would have a correlation coefficient of 1.0, a slope of 1:1, and a zero intercept.

9.5 MANAGEMENT APPLICATIONS

Once the model is calibrated and validated, it can be used to simulate future conditions to determine effects of changes in waste loads or to investigate causes of existing problems. This section describes three types of management application: (1) load-response analysis, (2) determination of acceptable nutrient loads, and (3) investigation of causes of nutrient problems.

Load-Response Analysis

A load-response analysis consists of performing multiple model simulations using different loading rates and examining the water quality predicted for each simulation. The most common use of a model to investigate nutrients in estuaries is to determine the water quality throughout an estuary in response to changes in nutrient loads. Models are designed to predict water quality based on loadings and environmental conditions (Figure 9-2).

This type of analysis also requires specification of the environmental conditions (e.g., freshwater inflows, tidal conditions) to be considered. The results of the load-response analysis are directly related to the

environmental conditions specified for the model simulation. For example, use of summer-average environmental conditions in the model will show the response in summer-average water quality to changes in loads. For the simplest Level I models, environmental conditions are specified implicitly through the use of salinity observations. Predictions from these models will correspond to the environmental conditions that were in effect when the salinity was measured. The more complex models require explicit definition of environmental condition and can be used to provide predictions for a wide range of environmental conditions.

Acceptable Nutrient Loads

The most common use for water quality models is to define allowable loads necessary to achieve water quality objectives. As seen in Figure 9-2, models predict water quality for a specified set of loads and environmental conditions. Determination of acceptable loads typically requires an iterative procedure, as shown in Figure 9-3. The first iteration consists of performing a model simulation using existing loads and comparing predicted water quality with objectives. Assuming that the existing loads result in unacceptable water quality, additional model simulations are performed using incremental reductions in nutrient loads until water quality objectives are achieved.

The approach shown in Figure 9-3 can be used to define necessary reductions in total loads as well as reductions in individual contributors to the total load.

The results of the above approach are highly dependent on the environmental conditions selected, as allowable loading rates can vary substantially across different environmental conditions. Two approaches are available for selecting critical conditions for use in defining allowable loads. These approaches are termed the critical conditions approach and the continuous simulation approach. In the critical conditions approach, a single set of environmental conditions is selected for analysis. These conditions typically represent critical or worst-case conditions, that is, those environmental conditions that will result in the poorest water quality for a given set of loads. The rationale for the critical conditions approach assumes that if loads are defined to meet water quality objectives during “critical” conditions, the same loads will result in attaining water quality objectives during most other conditions as well.

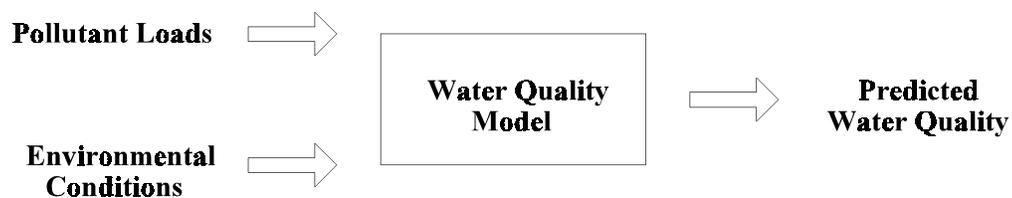


Figure 9-2. Use of models in load-response analysis.

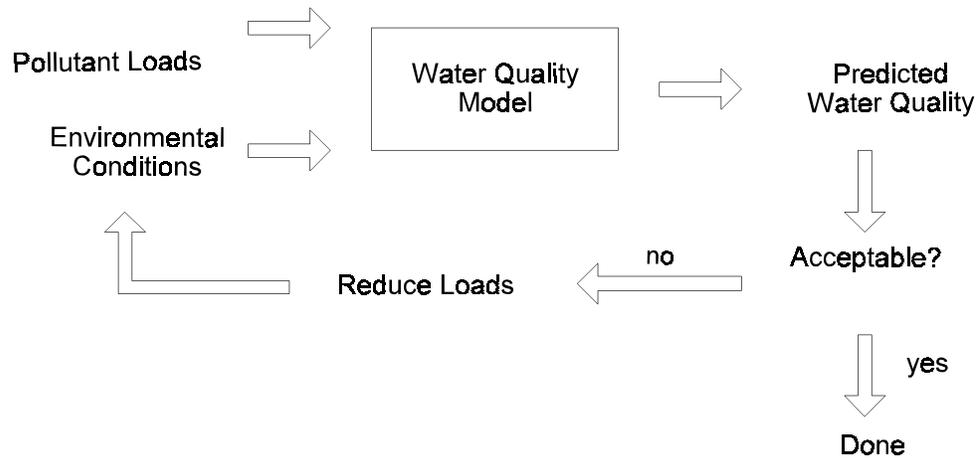


Figure 9-3. Use of models in determining allowable loads.

The continuous simulation approach performs simulations for as long a duration as is feasible, using historically observed variations in environmental conditions. The predicted water quality resulting from the continuous simulation is analyzed to determine the frequency with which water quality problems are observed to occur.

The overall intent of the modeling analysis is to define loads that will restrict the occurrence of water quality problems to an acceptable frequency. Each of the above two methods has particular strengths and weaknesses for performing this task. The continuous simulation approach provides a direct means to consider frequency of occurrence (i.e., number of years per problem) but has extreme resource requirements. The ability to perform continuous simulation of sufficient duration typically is constrained by the availability of data describing historical environmental conditions, or by computational requirements for the higher level models. The critical conditions approach has much more manageable resource requirements; however, there are no clear methods to establish appropriate critical conditions. In estuaries, freshwater, tides, wind, and other factors all can affect water quality. Selection of appropriate values for each environmental parameter requires considerable judgment. Furthermore, the specific level of protection associated with any single set of environmental conditions cannot be evaluated without performing a continuous simulation.

Case Study Example

Water quality models also can be used to gain an increased understanding of the relative importance of various loading sources to an estuary or near-coastal water. It is possible to investigate the contribution of individual loading sources to the water quality problem by performing a series of simulations examining each loading source separately. Because most water quality models assume a linear relationship between pollutant load and resulting water quality impact, it is possible to determine overall impacts to the estuary by summing the impacts from each source.

Investigation of Causes of Nutrient Problems

Shippo Creek (Figure 9-4) is a long, narrow, tidal tributary receiving nutrient inputs from upstream runoff and a single wastewater treatment plant (WWTP). This case study example demonstrates the use of models to perform three tasks:

- Estimate the contribution of various loading sources to the overall summer-average total nitrogen concentration
- Estimate the effect of a 50% reduction in loads from the WWTP on total nitrogen concentrations throughout the estuary
- Estimate the reduction in loading necessary to achieve an average total nitrogen concentration of 0.100 mg/L in the lower half of the estuary

Short-term answers were required, and screening-level accuracy was judged acceptable because of the short timeframe and limited data available.

The Fraction of Freshwater Method was selected because the estuary was considered one-dimensional, long-term average results were acceptable, and the water quality target was specified in terms of total nutrient levels.

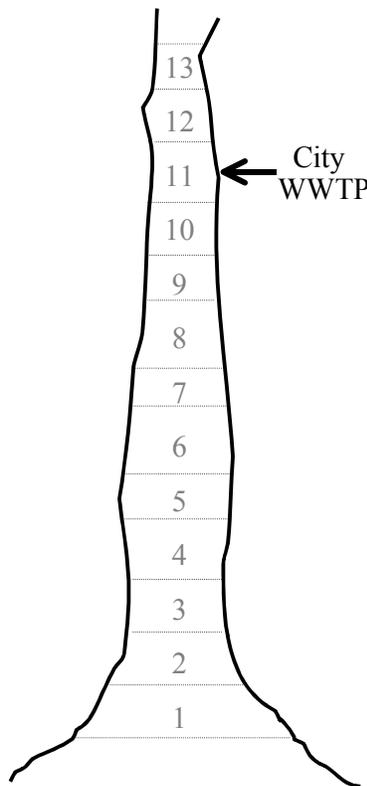


Figure 9-4. Shippo Creek site map and salinity monitoring location.

Information available to support the study included summer-average salinity measurements at 13 locations along the length of the estuary, summer-average freshwater inflows and total nitrogen loads to the estuary, nitrogen loads from the WWTP, and nitrogen and salinity concentrations outside of the estuary. This information was compiled as shown in Table 9-3 to allow implementation of the Fraction of Freshwater Method. The top two rows of Table 9-3 show the measured loading rates and seaward boundary conditions. The two leftmost columns define segments centered around each of the salinity measurements. The third column applies Equation 9-1 to calculate the fraction of freshwater in each segment.

The fourth through sixth columns in Table 9-3 apply Equations 9-2 or 9-3 as appropriate to determine the incremental contribution to the total nitrogen (TN) concentrations from each of three possible contributing sources: upstream (TN_{UP}), wastewater treatment plant (TN_{WWTP}), and the downstream seaward boundary (TN_{SEA}). Equation 9-2 is applied only to those segments downstream of the loading source, whereas Equation 9-3 is applied to those segments upstream of the loading source. Equation 9-2 is applied to all segments for examining impacts from upstream sources, whereas Equation 9-3 is applied to all segments for examining impacts from the seaward boundary. For determining WWTP impacts, Equation 9-2 is applied to segments 1-11 and Equation 9-2 is applied to segments 12-13. The final column in Table 9-3 sums the incremental contributions from each of the sources to provide a prediction of overall TN concentrations throughout the estuary.

Table 9-3. Calculation spreadsheet for Shipp's Creek estuary

Freshwater Inflow		Seawater Salinity	Upstream Load	WWTP Load	Seawater TN	
Q = 100,000 cmd		S_s = 30 ppt	W = 5,000 g/day	W = 500,000 g/day	0.005 ppm	
Segment #	Salinity, S _i (ppt)	Fraction of Freshwater, f _f	TN _{UP} (mg/L)	TN _{WWTP} (mg/L)	TN _{SEA} (mg/L)	Overall TN (mg/L)
1	29	0.03	0.002	0.017	0.005	0.023
2	27	0.10	0.005	0.050	0.005	0.060
3	25	0.17	0.008	0.083	0.004	0.096
4	23	0.23	0.012	0.117	0.004	0.132
5	21	0.30	0.015	0.150	0.004	0.169
6	19	0.37	0.018	0.183	0.003	0.205
7	18	0.40	0.020	0.200	0.003	0.223
8	16	0.47	0.023	0.233	0.003	0.259
9	14	0.53	0.027	0.267	0.002	0.296
10	12	0.60	0.030	0.300	0.002	0.332
11	10	0.67	0.033	0.333	0.002	0.368
12	5	0.83	0.042	0.110	0.001	0.152
13	1	0.97	0.048	0.025	0.000	0.074

The results of this modeling analysis are shown graphically in Figure 9-5, showing the overall TN distribution as well as its component. Although the Fraction of Freshwater Method does not require calibration, it would be worthwhile at this point to confirm that the model predictions of TN throughout the estuary were consistent with observed data collected over the same time period. Figure 9-5 shows that the WWTP is the dominant source of nitrogen throughout most of the estuary. Upstream sources are the dominant component only at the extreme head of the estuary. Nitrogen contributions from the seaward boundary are small throughout the system. The results in Table 9-2 and Figure 9-4 satisfy the first objective of this study, which was to determine the contribution of various loading sources to the overall summer-average total nitrogen concentration. The second objective of the study was to determine the water quality resulting from a 50% reduction in WWTP TN loads. This was accomplished by reapplying Equations 9-2 and 9-3 using one-half of the original WWTP loads. Results of this analysis are shown in Figure 9-6, indicating a decrease in peak TN concentrations from 0.368 to 0.202 mg/L and a decrease in lower estuary (defined as segments 1-6) average concentrations from 0.111 to 0.064 mg/L. This nearly 50% reduction in concentrations was expected, because the original analysis had demonstrated that the WWTP was the dominant loading source to the estuary.

The final objective of the study was to determine the loading reductions necessary to achieve a lower estuary average concentration of 0.08 mg/L. No single answer exists to this question, because three separate sources of nitrogen to the estuary contribute to the total concentration. Analysis of the data in Table 9-3 shows that the incremental contribution of the upstream, WWTP, and seaward sources to lower estuary average concentrations were 0.010, 0.100, and 0.004 mg/L, respectively. Because the seaward

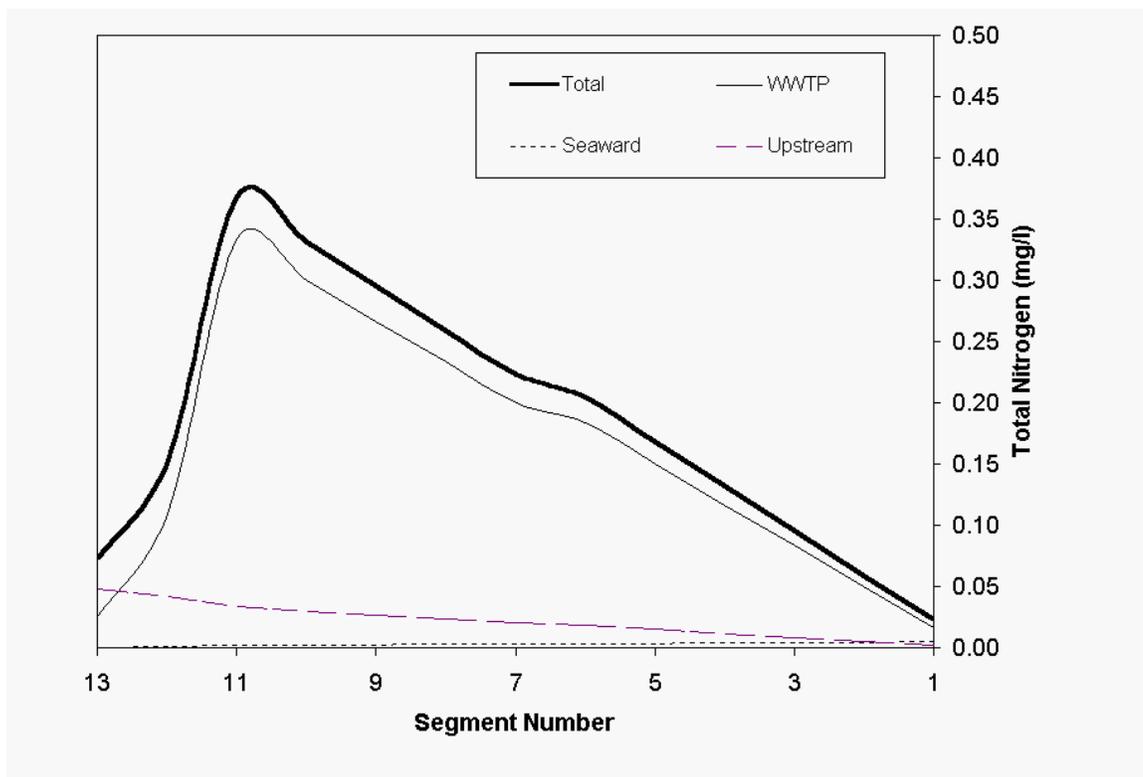


Figure 9-5. Model results for existing conditions.

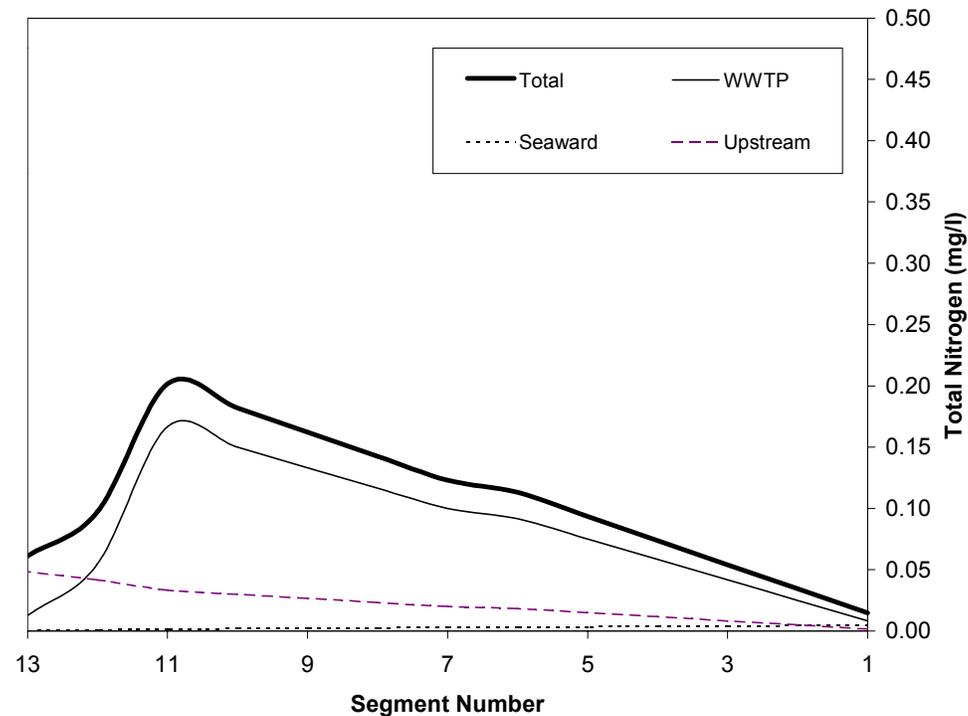


Figure 9-6. Model results for 50% reduction in WWTP load.

boundary nitrogen concentration cannot be controlled, management reductions must be restricted to either the upstream sources or the WWTP. The WWTP load must be reduced by at least 20% to meet the target TN concentration of 0.080 mg/L; otherwise, its contribution alone will exceed the target. Beyond the initial 20% reduction in the WWTP source, further reductions must come either from the WWTP or upstream sources. The specific allocation of these load reductions among sources is an economic and social decision that the model is not designed to address. The model is expressly designed, however, to test alternative proposals of load reductions to determine if they will meet the water quality objective. For example, a 25% reduction in both upstream and WWTP sources resulted in an average concentration of 0.087 mg/L (i.e., above the target), but a 30% reduction in WWTP loads coupled with a 40% reduction in upstream loads was shown to just meet the target.

All model simulations presented here should be viewed with extreme caution, because they are based on an uncalibrated, screening-level model. The level of uncertainty for these predictions cannot be quantified and is expected to be quite large. The model results do, however, provide the best possible estimate describing the relationship between nutrient loads and resulting concentrations, given the available resources.

Overview of Chesapeake Bay Airshed, Watershed, and Estuary Models

The cross-media models used in the Chesapeake Bay analysis consist of three models: an airshed model, a watershed model, and a model of the Chesapeake estuary. These models are linked so that the output of one simulation provides input data for another. The simulation period is the 10-year period of January

1, 1985, to December 31, 1994. Versions of these models have been used by the Chesapeake Bay Program for more than a decade and have been refined and upgraded several times.

Airshed Model

The Chesapeake Bay Program airshed model provides estimates of atmospheric deposition loads of nitrogen. A product of the EPA National Exposure Research Laboratory in Research Triangle Park, North Carolina, RADM (pronounced “radum”) is an acronym for Regional Acid Deposition Model. RADM is a three-dimensional model that tracks nutrient emissions across the eastern United States. Two RADM grids meet various resolution needs. A large grid scale covers the entire RADM domain and contains 20,000 square cells of 6,400 square kilometers each. A fine grid scale covers the region of the Chesapeake Bay watershed and has 60,000 cells, each covering 400 square kilometers. The model domain in the vertical is 15 cells deep, reaching from ground level to the top of the free troposphere. The depth of the cells increases with altitude. One of the findings of the RADM model is that the Chesapeake Bay airshed, defined as the area accounting for 75% of the deposition in the watershed, is approximately 5.5 times the size of the watershed.

RADM is used to drive scenarios associated with reductions in atmospheric deposition of nitrogen. A base condition deposition represents an estimate of the current condition of atmospheric deposition in the watershed and is developed from a regression of National Atmospheric Deposition Program (NADP) data. RADM scenarios of atmospheric deposition reductions are incorporated into Watershed Model scenarios by adjusting the base NADP condition on a segment-by-segment basis with a percent change prescribed by RADM scenario results. Results from RADM specify loads of wet and dry deposition to the Chesapeake watershed for the State Implementation Program (SIP) and Limit of Technology scenarios. Deposition loads are input directly to the land surfaces of the watershed model or to the tidal water surface of the Chesapeake Bay estuary model package as daily loads of wet deposition (from rain washout of atmospheric nitrate and ammonia) and 12-year average loads of dry deposition.

Three atmospheric deposition loads were used for the Chesapeake analysis: (1) the base condition of atmospheric deposition, (2) the estimated atmospheric deposition of nitrogen equivalent to the 1998 SIP controls of atmospheric deposition, and (3) the estimated atmospheric deposition under full limit of technology control (see Table 9-4).

Table 9-4. Chesapeake watershed nitrogen deposition under varying management schemes for emissions of nitrogen atmospheric deposition precursors

Scenario	TN Deposition (millions of kg/year)
Base Condition	204
State Implementation Plan (SIP)	178
Limit of Technology	128

Sources: Chesapeake Bay Program Phase IV Watershed Model and RADM.

Watershed Model

The watershed model simulates nutrient and sediment loads delivered to the Chesapeake Bay from all areas of the watershed. Land uses of cropland, pasture, urban areas, and forests are simulated on an hourly time-step, tracing the fate and transport of input nutrient loads from atmospheric deposition, fertilizers, animal manures, and point sources. The simulation is an overall mass balance of nitrogen and phosphorus nutrients in the basin, so that the ultimate fate of input nutrients is simulated, either as incorporation into crop or forest plant material, incorporation into soil, or river runoff. Nitrogen fates included volatilization into the atmosphere and denitrification. Transport in rivers is simulated to the tidal waters of the Chesapeake Bay. Sediment is simulated as eroded material washed off land surfaces and transported to the tidal bay. Scenarios are run for 10 years on a 1-hour time-step, and results are aggregated into 10-year average loads for comparison among scenarios.

To simulate the delivery of nutrients and sediment to the bay, the watershed was divided into 86 major model segments, each with an average area of 194,000 hectares. Segmentation, based on three tiers of criteria, partitioned the watershed into regions of similar characteristics. The first criterion was segmentation of similar geographic and topographic areas, which were further delineated in terms of soil type, soil moisture holding capacity, infiltration rates, and uniformity of slope. The second criterion involved finer segmentation based on spatial patterns of rainfall. Each segment had a bank-full travel time of about 24–72 hours. The third criterion used to further delineate segments was based on features of the river reach. River reaches containing a reservoir were separated into a reservoir simulation and a river simulation of the free-flowing river. For example, the James basin had 11 model segments, 2 represented reservoirs on the James and Appomattox, and the segmentation generally became finer with closer proximity to tidal waters.

Model segments were located to take advantage of observed data locations, so that a model segment outlet was located close to monitoring stations. Water quality and discharge data were collected from Federal and State agencies, universities, and other organizations. More than 150 subsegments were used at the interface between the watershed and estuary models to accurately deliver flow, nutrient, and sediment loads to appropriate areas of the estuary. Increased simulation accuracy motivated the division of basins into multiple segments and into simulation time-steps of an hour, but all scenario results were reported at the level of the basin and for 10-year average loads.

The watershed model has been in continuous operation at the Chesapeake Bay Program since 1982 and has had many upgrades and refinements since that time. The watershed model used for this application was Phase 4.1 based on the HSPF Version 11 code (Hydrologic Simulation Program - Fortan - HSPF). Version 11 is a widely used public domain model supported by EPA, USGS, and the U.S. Army Corps of Engineers.

Estuary Model

The Chesapeake Bay Estuary Model Package (CBEMP) is actually several models simulating different aspects of water quality in the bay and tributaries. A water quality model simulates 22 parameters, or state variables, as listed in Table 9-5.

Table 9-5. Water quality state variables used in CBEMP

Temperature	Dissolved organic nitrogen
Salinity	Labile particulate organic nitrogen
Inorganic suspended sediments	Refractory particulate organic nitrogen
Diatoms	Total phosphorus
Cyanobacteria (blue-green algae)	Dissolved organic phosphorus
Other phytoplankton	Labile particulate organic phosphorus
Dissolved organic carbon	Refractory particulate organic phosphorus
Labile particulate organic carbon	Dissolved oxygen
Refractory particulate organic carbon	Chemical oxygen demand
Ammonium	Dissolved silica
Nitrate + nitrite	Particulate biogenic silica

Zooplankton were separated into two size classes: microzooplankton (>44 microns) and mesozooplankton (>202 microns).

Linked to the water quality model is a hydrodynamic model, simulating the hydrodynamics, or water movement, throughout the tidal estuary. The hydrodynamic model produced three-dimensional predictions of velocity, diffusion, surface elevation, salinity, and temperature on an intratidal time scale. The model grid of the hydrodynamic and water quality models consists of more than 10,000 cells.

The modeling process involves simulation of living resource parameters, such as dissolved oxygen, chlorophyll concentrations, and submerged aquatic vegetation (SAV). Computed parameters are compared with living resource standards, and an estimation is made of the degree to which computed conditions benefit the resources of interest (e.g., fish, oysters). In addition, the CBEMP includes the direct interactive simulation of SAV and water quality. Three phytoplankton groups were simulated.

Over seasonal time scales, the bay sediments are a significant source of dissolved nutrients to the overlying water column. The role of sediments in the systemwide nutrient budget is especially important in summer when seasonal low flows diminish riverine nutrient input. In addition, water temperatures enhance biological processes in the sediments, creating greater sediment oxygen demand. Bay sediments retain a long-term nutrient load “memory” of several years; that is, sediment nutrient fluxes to the water column are determined by organic nutrient inputs from several previous years. Therefore, the water quality model was coupled directly to a predictive benthic-sediment model. These two models interact at each time-step, with the water quality model delivering settled organic material to the sediment bed, and the benthic-sediment model calculating the flux of oxygen and nutrients to the water column.

Linked to the CBEMP are the watershed and airshed models, which provide daily input data. Generally, 10-year scenarios are run on 15-minute time-steps with output generated each 10 days. The estuary

model has been in operation since 1987, with two major model refinements released since the initial 1987 steady-state model.

Further information on the entire suite of Chesapeake Bay Program models, their documentation, and application can be found at: <http://www.chesapeakebay.net/model.htm>.