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A Dynamic Water-Quality Modeling Framework for the Neuse River Estuary, North Carolina

U.S. Geological Survey
Water-Resources Investigations Report 99–4017

U.S. Department of the Interior
U.S. Geological Survey

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By JERAD D. BALES and JEANNE C. ROBBINS

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Raleigh, North Carolina
1999

U.S. DEPARTMENT OF THE INTERIOR
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CONVERSION FACTORS, TEMPERATURE, VERTICAL DATUM, AND DEFINITIONS

Multiply	By	To obtain
	Length	
centimeter (cm)	0.394	inch
meter (m)	3.281	foot
kilometer (km)	0.6214	mile
	Area	
square meter (m^2)	10.76	square foot
square kilometer (km^2)	0.3861	square mile
	Volume	
liter (L)	0.2642	gallon
cubic meter (m^3)	35.31	cubic foot
cubic meter (m^3)	264.2	gallon
	Flow rate	
cubic meter per second (m^3/s)	35.31	cubic foot per second
meter per second (m/s)	3.281	foot per second
	Mass	
gram (g)	0.03527	ounce, avoirdupois

Temperature in degrees Celsius (°C) may be converted to degrees Fahrenheit (°F) as follows:

$$°F = (1.8 \times °C) + 32$$

Sea level: In this report, "sea level" refers to the National Geodetic Vertical Datum of 1929 (NGVD of 1929)—a geodetic datum derived from a general adjustment of the first-order level nets of both the United States and Canada, formerly called Sea Level Datum of 1929.

Specific conductance is given in microsiemens per centimeter (µS/cm) at 25 degrees Celsius.

Concentrations of chemical constituents in water are given either in milligrams per liter (mg/L) or micrograms per liter (µg/L).

A Dynamic Water-Quality Modeling Framework for the Neuse River Estuary, North Carolina

By Jerad D. Bales and Jeanne C. Robbins

ABSTRACT

As a result of fish kills in the Neuse River estuary in 1995, nutrient reduction strategies were developed for point and nonpoint sources in the basin. However, because of the interannual variability in the natural system and the resulting complex hydrologic-nutrient interactions, it is difficult to detect through a short-term observational program the effects of management activities on Neuse River estuary water quality and aquatic health. A properly constructed water-quality model can be used to evaluate some of the potential effects of management actions on estuarine water quality. Such a model can be used to predict estuarine response to present and proposed nutrient strategies under the same set of meteorological and hydrologic conditions, thus removing the vagaries of weather and streamflow from the analysis.

A two-dimensional, laterally averaged hydrodynamic and water-quality modeling framework was developed for the Neuse River estuary by using previously collected data. Development of the modeling framework consisted of (1) computational grid development, (2) assembly of data for model boundary conditions and model testing, (3) selection of initial values of model parameters, and (4) limited model testing.

The model domain extends from Streets Ferry to Oriental, N.C., includes seven lateral embayments that have continual exchange with the mainstem of the estuary, three point-source discharges, and three tributary streams. Thirty-five computational segments represent the mainstem of the estuary, and the entire framework contains a total of 60 computational segments. Each computational cell is 0.5 meter thick; segment lengths range from 500 meters to 7,125 meters.

Data that were used to develop the modeling framework were collected during March through October 1991 and represent the most comprehensive data set available prior to 1997. Most of the data were collected by the North Carolina Division of Water Quality, the University of North Carolina Institute of Marine Sciences, and the U.S. Geological Survey.

Limitations in the modeling framework were clearly identified. These limitations formed the basis for a set of suggestions to refine the Neuse River estuary water-quality model.

INTRODUCTION

A series of dramatic and extensive fish kills occurred in the Neuse River estuary (fig. 1) in the summer of 1995. Outbreaks of the dinoflagellate *Pfiesteria piscicida* also were reported. Citizens complained of a variety of health problems resulting from contact with water from the Neuse River. However, it also has been widely recognized that the Neuse River estuary had experienced large, and possibly increasing, nitrogen loadings for some time prior to 1995 (Paerl and others, 1995).

Although unusual precipitation and temperature patterns in the spring and summer of 1995 likely contributed to the extreme conditions in the Neuse River estuary, public outcry for action to correct perceived problems was overwhelming. A special

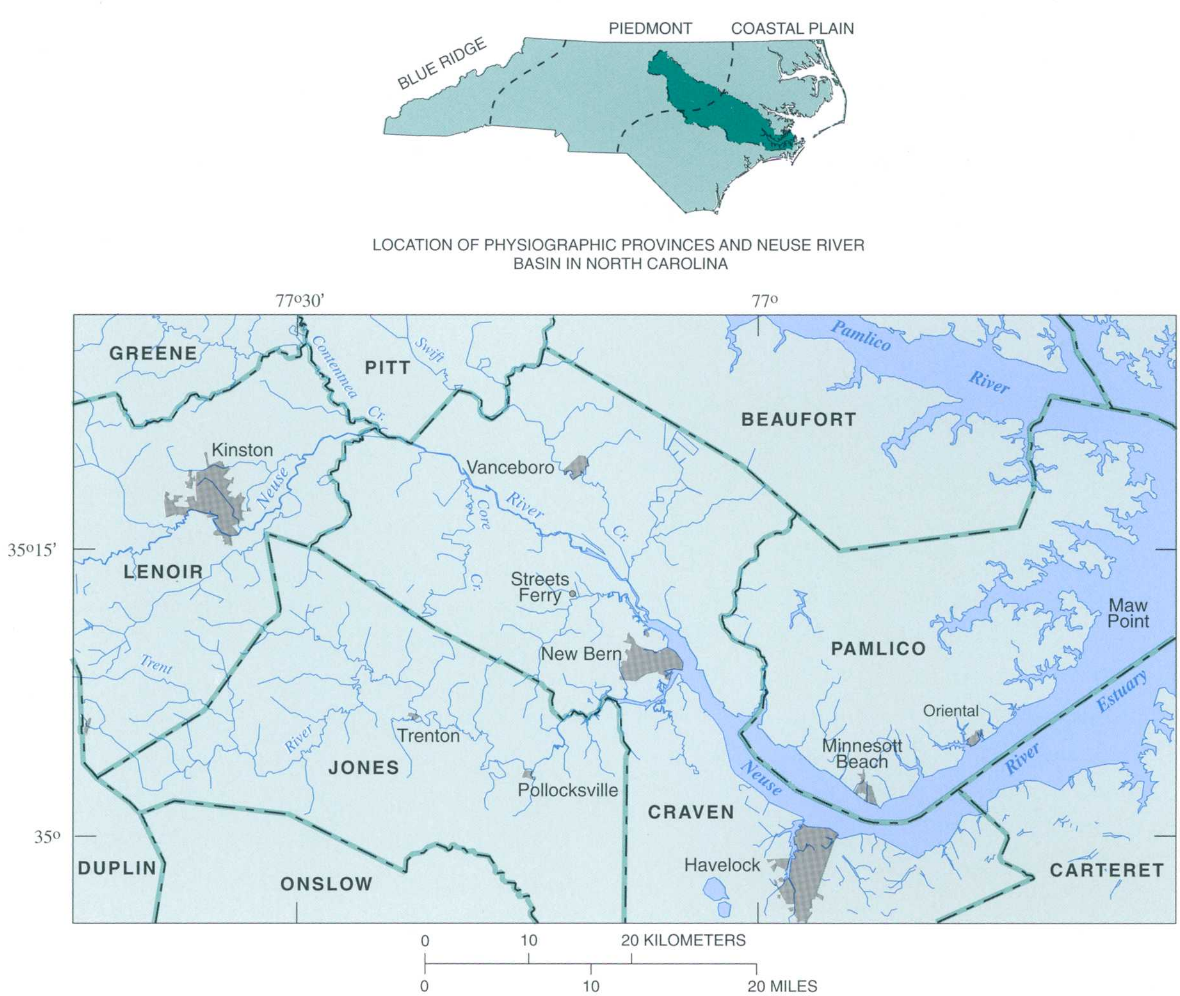


Figure 1. The Neuse River from Kinston to the mouth of the estuary at Pamlico Sound, and the Neuse River Basin in eastern North Carolina.

legislative committee was formed to recommend solutions, scientists and citizens met repeatedly to address issues, and the North Carolina General Assembly committed funds to improve water quality in the estuary.

As a result of the events in the Neuse River estuary in 1995, nutrient reduction strategies were developed for point and nonpoint sources in the basin. However, the effects of these strategies are difficult to assess directly because of the confounding influences of weather, hydrology, diverse sources of nutrient inputs to the estuary, and complex hydrologic nutrient interactions. For example, dissolved-oxygen (DO) concentrations of less than 3 mg/L can occur throughout the year in parts of the estuary, but the causes for the low levels are not fully understood (Garrett and Bales, 1991; Garrett, 1992, 1994). Bottom sediments apparently exert a large oxygen demand on the water column (Jay Sauber, North Carolina Division of Water Quality, oral commun., April 1998) and seem to be a continuing source of nutrients to the estuary (Haruthunian, 1997).

Three important hydrologic-nutrient interactions that are strong determinants of the amounts and types of phytoplankton production in the lower Neuse River and estuary were identified in previous studies (Christian and others, 1985; Paerl, 1987; Paerl and others, 1990, 1995; and Mallin and others, 1993). These interactions are (1) river flow and water residence time in the estuary; (2) timing and magnitude of nitrogen loading, as well as the ratio of nitrogen to phosphorus concentrations; and (3) salinity regime, including the vertical and longitudinal distribution of salinity in the estuary.

Because of the interannual variability in the natural system and the resulting complex hydrologic-nutrient interactions, it is difficult to detect through a short-term observational program the effects of management activities on Neuse River estuary water quality and aquatic health. However, a properly constructed water-quality model can be used to evaluate some of the potential effects of management actions on estuarine water quality. Such a model can be used to predict estuarine response to present and proposed nutrient strategies under the same set of meteorological and hydrologic conditions, thus removing the vagaries of weather and streamflow from the analysis.

In 1996, the North Carolina Division of Water Quality (DWQ) and the U.S. Geological Survey (USGS) began a cooperative effort to develop a two-dimensional, laterally averaged hydrodynamic and water-quality modeling framework for the Neuse River estuary. The modeling framework was developed by using previously collected data—no new data were collected during the study. Moreover, the DWQ and USGS recognized that all required data were not available to develop the model, and that some information would have to be estimated from available data. However, the study objective, which was to develop a modeling framework that could be enhanced by using a more complete data set, was met.

Purpose and Scope

The purpose of this report is to document the development of the first phase of a water-quality modeling framework for the Neuse River estuary. Included in the documentation are (1) a brief overview, including major assumptions and limitations, of the water-quality model around which the framework was developed; (2) presentation of the computational grid for the model; (3) discussion of the data used for model boundary conditions and model testing; and (4) summary of model capabilities and limitations, as well as possible future refinements and appropriate applications of the model.

The model CE-QUAL-W2 (Cole and Buchak, 1995), which is a laterally averaged, hydrodynamic and water-quality model, was used to develop the framework. The computational grid for the model extends from Streets Ferry to Oriental (fig. 1) along the mainstem of the estuary, and includes seven embayments. Data that were used for the modeling framework were collected primarily during 1991. Data from this period represented the most comprehensive data set available at the time the modeling framework was being developed.

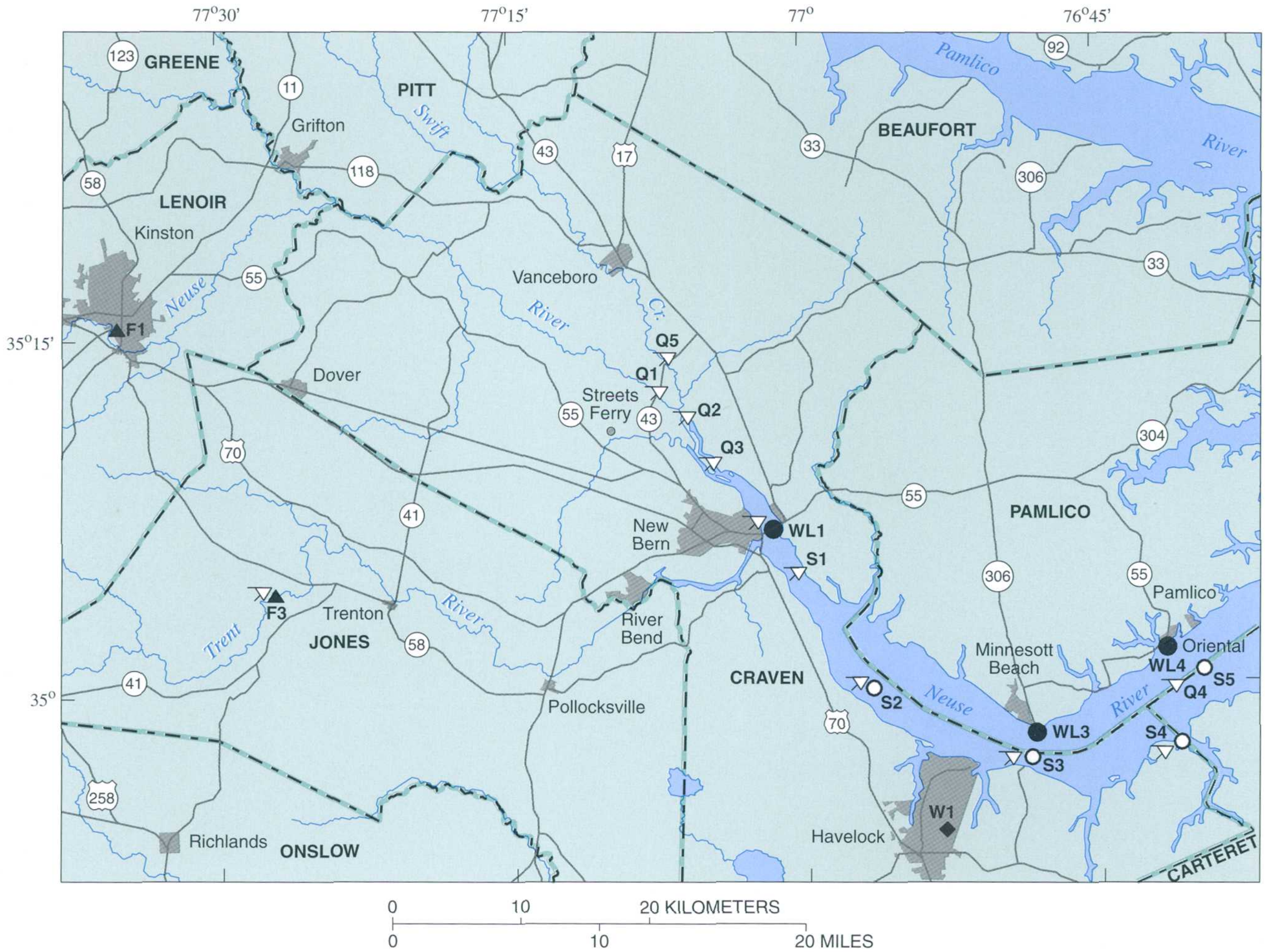
In 1997, the DWQ awarded the Water Resources Research Institute (WRRI) of the University of North Carolina a grant to conduct monitoring and modeling in the Neuse River estuary. The Neuse River estuary water-quality modeling framework described in this report was transferred to the WRRI team. Since that time, the model has been tested and significantly modified (J.D. Bowen, The University of North Carolina at Charlotte, oral commun., April 1998). Modifications include changes to the computational grid and the addition of several new algorithms to enhance capabilities of the model. Moreover, the WRRI team and others (DWQ, Weyerhaeuser Company, and the USGS) collected a fairly comprehensive hydrodynamic and water-quality data set during the summer and fall of 1997. These data should facilitate extensive calibration and testing of the revised and enhanced version of the Neuse River water-quality model.

Physical Setting

The model domain (or study area) includes the Neuse River from Streets Ferry to the mouth of the Neuse River estuary near Oriental (fig. 2). Also included in the study area are parts of seven tributaries, including the Trent River.

Much of the shoreline surrounding the Neuse River estuary is composed of marshes, particularly near the mouth of the estuary. However, high (3- to 5-m) bluffs predominate along the south shore of the estuary between New Bern and Cherry Point (Bellis and others, 1975). Elevations of land surfaces that drain directly to the study area are generally less than 8 m above sea level. Streams that drain directly to the estuary have small drainage areas, little topographic relief, low sediment loads, and fairly acidic waters.

Prior to 1997, the downstream-most streamflow gaging station on the Neuse River was located at Kinston, where the drainage area is 7,010 km^2. In comparison, the drainage area at New Bern is 11,620 km^2, and 14,547 km^2 at the mouth of the estuary. Flows in the Neuse River have been regulated by Falls Dam since 1983, but the drainage area upstream from Falls Dam is only 2,010 km^2, or less than 20 percent of the total drainage area at New Bern. The annual mean flow at Kinston during 1983–96 was 78 m^3/s, and the highest flow at Kinston was after



EXPLANATION

- W1 ◆ METEOROLOGICAL STATION AND NUMBER
- S1 ▽ PHYSICAL, CHEMICAL, AND BIOLOGICAL SAMPLING SITE AND NUMBER
- F1 ▲ STREAMFLOW STATION AND NUMBER
- S5 ○ TEMPERATURE, SALINITY, AND DISSOLVED OXYGEN STATION AND NUMBER
- WL3 ● WATER LEVEL STATION AND NUMBER

Figure 2. The Neuse River estuary from Streets Ferry to the mouth showing streamflow, water level, temperature/salinity/dissolved-oxygen concentration monitoring locations, wind station, and water-quality sampling locations.

Hurricane Fran in 1996, when the flow reached 770 m^3/s. Flows during the 5-year period 1988–92 were extremely low at Kinston, and the only periods of sustained higher-than-normal flows between 1988 and 1997 were during November 1992 through April 1993, June 1995 through February 1996, and September 1996 through February 1997.

Water-level fluctuations in the Neuse River estuary often exhibit a marked periodicity (Robbins and Bales, 1995), although these fluctuations probably are not driven by astronomical tides (Jarrett, 1966; Pietrafesa and others, 1986). Low frequency fluctuations in Neuse River estuary water levels are forced by Pamlico Sound water levels, but a combination of the sea breeze effect or seiching of Pamlico Sound could cause higher frequency fluctuations (on the order of 12 hours). During 1988–92, the mean water level at New Bern was 0.243 m above sea level, and it was 0.204 m above sea level at Oriental. The mean daily water-level range was

0.292 m at New Bern and 0.186 m at Oriental. The highest recorded water level at New Bern during 1988–97 was 2.52 m above sea level during Hurricane Fran in 1996, and the lowest recorded value was 1.20 m below sea level in March 1993.

Saltwater can travel upstream as far as Streets Ferry in the Neuse River. (During the severe drought of 1954, and before construction of Falls Dam, a specific conductance of 673 $\mu S/cm^2$ was measured near Fort Barnwell, about 30 km upstream from New Bern; Giese and others, 1985.) Salinities at New Bern range from zero to about 10 ppt (parts per thousand) and can be as much as 30 ppt at Oriental (Garrett, 1994; Robbins and Bales, 1995). Salinity is typically the highest throughout the estuary during the summer. Stratification (the difference between top and bottom salinity) generally is much greater upstream from Cherry Point, although overall salinity is higher in the downstream segment of the estuary. Stratification is greatest during July and August but also can be high during January through April when inflows typically are high.

Currents in the Neuse River estuary exhibit complex spatial and temporal patterns. Robbins and Bales (1995) reported measurements of currents that were made continuously at 10 locations in the estuary for 18 days in 1989. Maximum current speeds ranged from 48 cm/s in the upstream direction to 52 cm/s downstream. Lateral asymmetry in the currents was observed at sections near Oriental and near Cherry Point. Wells and Kim (1991) reported that currents measured 1 m above the estuary bottom throughout a 30-km reach of the estuary and at monthly intervals were all directed in the upstream direction.

DO concentrations in the Neuse River estuary range from near zero to more than 150 percent of saturation. DO concentrations drop very quickly in the presence of density stratification, particularly during the summer and fall (Garrett, 1992). DO can remain less than 2 mg/L in bottom waters for several weeks during periods of high organic loading, such as after Hurricane Fran in September 1996, and during times of relatively stable stratification.

Paerl and others (1995) reported that DO concentrations of bottom waters at New Bern were less than 5 mg/L about 40 percent of the time when sampled between 1990 and 1993. Near-bottom DO concentrations of less than 5 mg/L occurred less than 10 percent of the time near the mouth of the estuary during the same period. However, Rizzo and Christian (1996) reported that sediment oxygen demand (SOD) did not vary spatially along the axis of the estuary. The mean SOD values from each of six sites, located between about Streets Ferry and the mouth of the estuary, were between 15.0 and 21.8 mg of oxygen/m^2/hr. The more frequent occurrence of density stratification in the upper reaches of the estuary partially explains the more frequent occurrence of lower DO concentrations in that area.

Concentrations of nitrate-nitrogen (NO_3), ammonium-nitrogen (NH_4), and orthophosphorus (PO_4) all generally decrease from upstream to downstream in the Neuse River estuary (table 1; Lebo, 1995; Paerl and others, 1995). During 1987–93, there were no consistent seasonal patterns in NO_3 and NH_4 concentrations, but PO_4 concentrations were generally higher in the summer than during other times of the year (Lebo, 1995; Paerl and others, 1995). However, Lebo (1995) observed that NO_3 concentrations varied with river flow, being higher during periods of high flow and lower during low-flow periods. Some top-to-bottom differences in NO_3 and PO_4 also were

Table 1. Mean and range (shown in parentheses) of concentrations of nitrate, ammonium, orthophosphorus, and chlorophyll *a* in the Neuse River estuary, 1987–93. Data from Paerl and others, 1995

[mg/L, milligram per liter; µg/L, microgram per liter]

Location (fig. 2)	Nitrate, in mg/L	Ammonium, in mg/L	Orthophosphorus, in mg/L	Chlorophyll *a*, in µg/L
New Bern	0.287 (0.034–0.618)	0.100 (0.010–0.371)	0.116 (0.034–0.217)	24 (0.7–148)
Near Adams Creek	0.026 (0.001–0.220)	0.045 (0.002–0.563)	0.051 (0.002–0.183)	16 (2–68)
Mouth of Neuse River estuary	0.009 (0.001–0.155)	0.019 (0.001–0.150)	0.043 (0.001–0.244)	11.4 (0.5–65)

observed. Productivity, as indicated by chlorophyll *a* concentrations, is greater in the upstream reach of the estuary than near the mouth (table 1).

Approach

The modeling approach consisted of (1) computational grid development, (2) assembly of data for model boundary conditions and model testing, (3) selection of initial values of model parameters, and (4) limited model testing. No new data were collected as part of the development of the water-quality modeling framework. Essentially all of the data that were used to develop the modeling framework were described by Garrett (1992, 1994), Paerl and others (1995), and Robbins and Bales (1995).

Some of the required boundary condition data, as explained subsequently, did not exist and were estimated from available data. Methods for estimating required information are described in this report. Likewise, adequate data for a complete model calibration were not available, so a rigorous model calibration was not performed. However, the first phase of the development of a water-quality modeling framework for the Neuse River estuary was successfully completed, and subsequent Neuse modeling efforts have been based on the first steps taken during this study.

Previous Studies

There have been numerous investigations of Neuse River estuary water-quality issues and somewhat fewer studies of hydrology and hydrodynamics of the estuary. However, investigations that resulted in calibrated and tested flow and(or) water-quality models for the Neuse River estuary are quite limited. This is likely because of the recognized complexity of the natural system, the difficulty in obtaining required data, and the long-term commitment required to develop a credible model.

Lung (1988) developed a tidally averaged, two-layer model of the Neuse River between Kinston and New Bern to simulate seasonal variations in salinity, nutrients, chlorophyll *a*, and DO concentrations. The study reach was divided into 13 longitudinal segments, and the model contained 11 water-quality constituents, including 4 algal groups. Although the model generally reproduced seasonal trends, agreement between simulation results and data generally was poor for any given time.

Weyerhaeuser Company contracted with Beak Consultants to develop a water-quality model for the Neuse River reach between approximately Streets Ferry and New Bern. The purpose of the model was to "serve as a link between the river loadings and the estuarine response" (North Carolina Division of Environmental Management, 1993). The model CE-QUAL-W2 was constructed and tested for the study reach. However, the model was not configured in a manner that allowed nutrients and algae concentrations to be simulated in a predictive mode, although CE-QUAL-W2 does have that capability.

Robbins and Bales (1995) constructed an unsteady, two-dimensional, vertically averaged hydrodynamic and solute transport model for the Neuse River estuary between New Bern and Oriental. The model was developed and extensively tested by using water level, salinity, velocity, and wind data that were collected by a fairly extensive data-collection network. The computational grid consisted of 5,800 200- x 200-meter computational cells. Bathymetry used to develop the grid was based on more than one million depth soundings in the estuary. Model results, as well as data, demonstrated the presence of lateral asymmetry in currents, including concurrent upstream and downstream flows at a section. Simulations also showed that under some conditions, material released in the estuary might not exit the estuary for more than 30 days. However, flows in the Neuse River estuary were demonstrated to be more dynamic than flows in the adjacent Pamlico River estuary (Robbins and Bales, 1994).

Acknowledgments

The assistance of Mr. Jon Mangles, formerly of the North Carolina Division of Water Quality, in assembling data for model input files is gratefully acknowledged. The support of Mr. Steve Tedder, formerly of the Division of Water Quality, and Ms. Ruth Swanek, Division of Water Quality, in initiating and continuing this investigation is greatly appreciated. Ms. Silvia Terziotti, USGS, provided valuable support in developing the computational grid for the modeling framework.

WATER-QUALITY MODELING FRAMEWORK

A two-dimensional, laterally averaged hydrodynamic and water-quality modeling framework was constructed for the Neuse River estuary. Data that were collected during March through October 1991 were used to develop boundary conditions required for model operation. The model has the capability to simulate water level, currents, heat and salt transport, and the transport and transformation of 10 chemical-physical constituents, algae, and temperature. Prediction of transport during stratified and unstratified conditions, the effects of the longitudinal salinity gradient on circulation (gravitational circulation), the effects of changing wind and air temperature on water-quality conditions, and the response of the estuary to changes in nutrient loadings can be accomplished through appropriate application of the modeling framework.

General Model Description

The planned primary application of the Neuse River estuary water-quality model is to realistically predict the effects of reductions in nitrogen inputs to the estuary on DO, nutrient, and algal concentrations in the estuary. Hence, a model that is capable of simulating the complex water movement and primary chemical processes that occur in an estuary is required. The tidal creeks that drain to the Neuse River estuary can be significant nutrient sources, and water-quality degradation is often seen in the embayments along the estuary. Consequently, the capability to predict transport and water-quality processes in these tidal creeks and embayments, including exchange with the mainstem, is needed. The primary gradients in physical, chemical, and biological conditions in the Neuse River estuary are fundamentally controlled by flow and by the vertical and longitudinal distribution of salt in the estuary. Although lateral gradients in salinity (Williams and others, 1967; Schwartz and Chestnut, 1973) and currents (Robbins and Bales, 1995) exist, these lateral gradients appear to be of secondary importance, relative to the vertical and longitudinal gradients, in controlling water-quality processes. Based on these requirements and because the CE-QUAL-W2 model is well documented and tested, and because of recent successful applications of the model by the USGS (Giorgino and Bales, 1997; Bales and Giorgino, 1998), the CE-QUAL-W2 model was selected for application to the Neuse River estuary.

The CE-QUAL-W2 model has been under continuous development since at least 1975 (Edinger and Buchak, 1975). Details on model theory and structure and a bibliography on theoretical development and applications are given by Cole and Buchak (1995).

Finite-difference forms of the complete unsteady, laterally averaged equations of conservation of mass, conservation of momentum, and transport (one equation for each constituent modeled) are solved within the model. Heat transport, salt transport, and momentum equations are dynamically coupled through the density gradient terms. The water movement affects the distribution of heat and salinity through advection and diffusion, and the heat and salinity distributions (primarily salinity) affect water movement through the presence of longitudinal and vertical density gradients. Likewise, heat transport and water quality are coupled because of the effects of suspended solids on light penetration and heat adsorption.

An efficient and accurate finite difference numerical scheme is used to solve the system of partial differential equations that describe flow and transport in the estuary. The appropriate maximum computational interval to ensure numerical stability is automatically computed for each time step in the simulation, so that the time step is variable throughout the simulation. The time step can be controlled somewhat by setting a maximum allowable value for the simulation.

The estuary is divided into a series of longitudinal segments, each of which may have a unique length (fig. 3). Branches also can be included so that complex estuarine morphologies, including tidal creeks, tributaries, and embayments, can be realistically represented by the computational grid. Each segment is further subdivided into layers. All layers within a segment must have the same length, but each layer can have a unique width and thickness (fig. 3). Conditions within each computational cell are assumed to be uniform, so that the governing equations are assumed to represent conditions throughout the cell. The cell-averaged longitudinal velocity, vertical velocity, density, temperature, and constituent concentrations are determined for each cell through the numerical solution of the governing equations; water-surface elevation is determined for the surface layer in each segment.

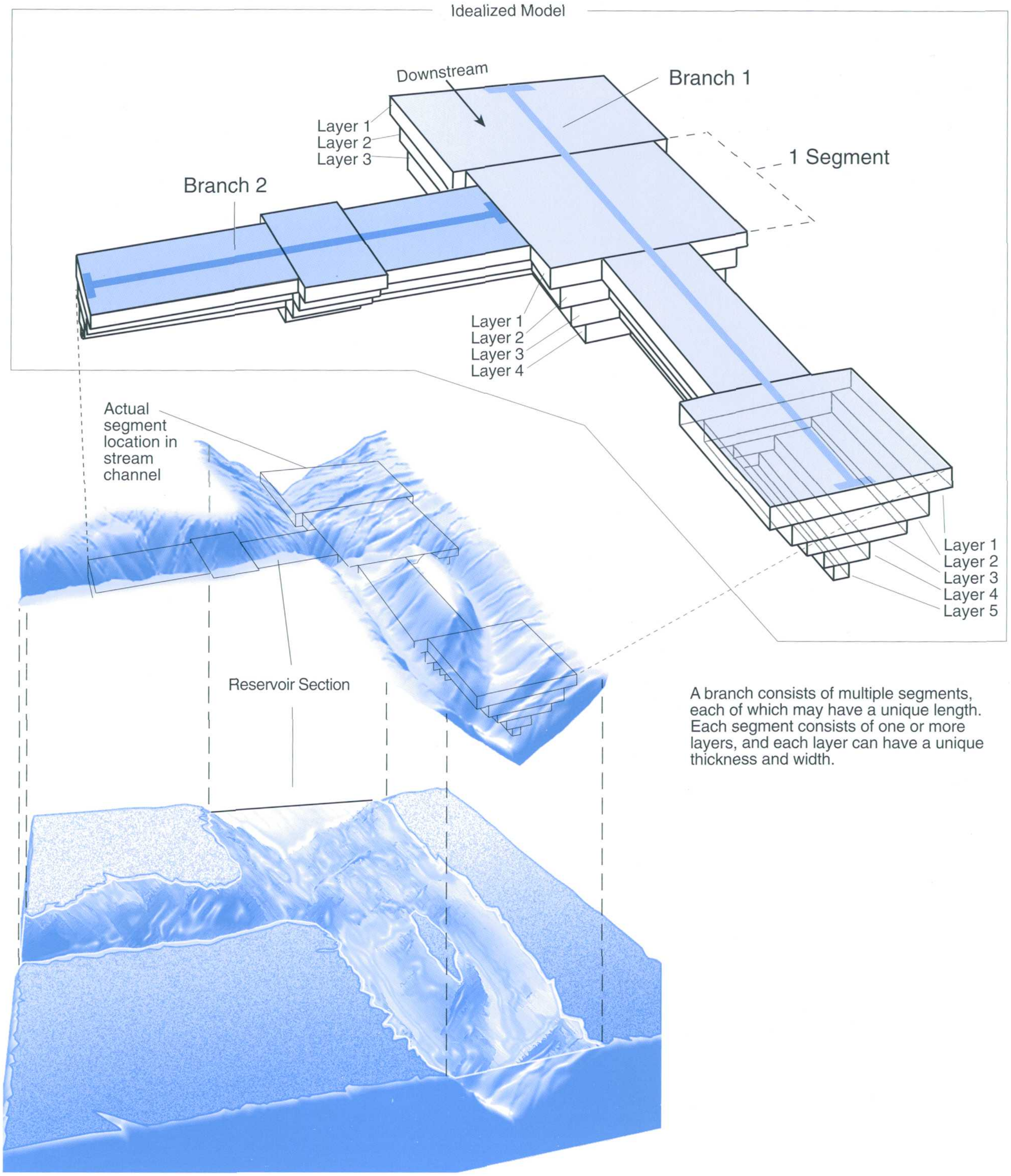


Figure 3. Idealized model segments, layers, and branches for a section of the Neuse River estuary.

Inflows to the estuary can occur at point sources, branches, or tributaries, which are treated like point sources into a segment. Outflows can occur at the downstream boundary or through withdrawals, none of which exist in the Neuse study area.

In addition to temperature, as many as 21 separate constituents can be included in the water-quality simulations, although only 10 constituents (in addition to temperature and salinity) are included in the Neuse River estuary model (table 2). Temperature and salinity must be included because of the dependence of flows on density gradients. Interdependence of the various constituents must be considered when selecting constituents for simulation.

In many systems, water-quality conditions vary more slowly than the hydrodynamics. Consequently, CE-QUAL-W2 allows the user to perform water-chemistry simulations at greater time steps than hydrodynamic calculations. However, in the Neuse River estuary, the water column can change from strongly stratified to unstratified in a matter of minutes (Robbins and Bales, 1995), and near-bottom DO can change from less than 1 mg/L to greater than 5 mg/L in less than 15 minutes (U.S. Geological Survey, unpublished provisional data, 1998). Hence, Neuse River estuary hydrodynamic and water-quality simulations may need to be performed at the same compuational time step.

Although CE-QUAL-W2 is quite rigorous in the treatment of hydrodynamics, heat transport, and chemical kinetics, the model does have limitations. These limitations need to be considered when applying the model and interpreting model results.

The estuary is assumed to be well mixed laterally at all points. Consequently, inflows from tributaries entering the estuary along one shoreline are assumed to

Table 2. Water-quality constituents included in the Neuse River estuary model

Constituent	Description
Conservative tracer	Neutrally buoyant, nonreactive material used for tracking water movement and determining water age.
Salinity	Affects density distribution and, thus, water movement.
Labile dissolved organic matter	Part of biological oxygen demand; consists of relatively fast decaying algal excretion and algae.
Refractory dissolved organic matter	Part of biological oxygen demand; slowly decaying compounds produced from decay of labile dissolved organic matter.
Algae	All phytoplankton are represented by one algal compartment; algae produce and use dissolved oxygen, utilize nitrate, ammonium, and phosphorus, and contribute to labile and refractory dissolved organic matter.
Detritus	Particulate organic material; decaying detritus exerts an oxygen demand in the water column and on the streambed, and is a source of nitrogen and phosphorus.
Phosphorus	Assumed to be completely available as orthophosphorus for use by algae; released by sediments under anoxic conditions; released by algal respiration and decay of organic matter.
Ammonium	Used by algae in photosynthesis; converted to nitrate under oxic conditions; released by sediments under anoxic conditions.
Nitrate-nitrite	Converted from ammonium (nitrification) under oxic conditions; lost from system by denitrification under anoxic conditions; used by algae.
Dissolved oxygen	Aerobic and anaerobic processes are simulated; dissolved oxygen lost by (1) decay of detritus and dissolved organic matter, (2) sediment oxygen demand, (3) nitrification processes, and (4) algal respiration; input by reaeration and algal photosynthesis.
Organic bottom sediments	Settling algae and detritus accumulate as organic bottom sediments; sediments decay, producing ammonium and phosphorus, and use dissolved oxygen.

be instantaneously mixed across the estuary at the point of entry to the estuary. In addition, inflows are instantaneously mixed longitudinally within the computational segment that the inflow enters.

The model has only one algal component, so algae succession cannot be simulated. Studies by Christian and others (1985) and Pinckney and others (1997) have shown that the types of algae present in the estuary change with the season and with salinity. Moreover, there are some indications that there may be a long-term shift in algal types with changes in nutrient loads. This is of particular importance when the shift is toward blue-green algae, which are not a good food source for zooplankton.

Chemical processes at the sediment-water interface are modeled rather simplistically by using either a zero- or first-order approximation. These processes may be particularly important, however, when evaluating the long-term effects of changes in external (point sources, tributaries, runoff, and atmospheric deposition) nutrient loadings on estuarine water quality. Processes at the sediment-water interface control internal loadings of nutrients to the estuary. These internal loadings appear to be a significant source of nutrients to the estuary (Haruthunian, 1997), but loadings from bottom sediments can change as a function of the external loading rate. The modeling framework does not simulate the effects of changes in external loadings on internal nutrient loads.

Modeling Framework

The modeling framework consists of the computational grid; boundary condition data, which are required for model operation; model parameters, which are set at some reasonable initial value and then adjusted during model testing; and selected other modeling options. These features are described in the following sections, with emphasis on the computational grid and boundary data.

Computational Grid

The model domain extends from Streets Ferry to near Oriental, or a distance of about 63 km. The domain includes 8 branches and a total of 60 active computational segments (table 3; fig. 4). The laterally averaged mathematical formulation of the numerical model suggests that the length of a particular computational segment should be greater than the maximum width of that segment. This is true for most of the segments in the Neuse River estuary model. Segment lengths varied from 500 to 7,125 m in length, and from 102 to 6,739 m in top width along the mainstem, or branch 1 (table 3). The number of active computational layers ranged from 4 to 27 (table 3), with each layer being 0.5 m thick. The orientation of the longitudinal axis of each segment relative to north was determined and used in the computation of surface wind stress for the segment.

Bathymetric data used by Robbins and Bales (1995) for the two-dimensional vertically averaged Neuse River estuary model were used to develop the computational grid for the water-quality model for the reach of the estuary between New Bern and Oriental. This reach included parts of branch 1, and branches 3–8. The original data were obtained from the National Ocean Survey (NOS) and were based on more than 1 million depth soundings. The original

Table 3. Description of the Neuse River estuary water-quality modeling framework computational grid
[m, meter]

Branch	Branch 1	Branch 2	Branch 3	Branch 4	Branch 5	Branch 6	Branch 7	Branch 8
Waterbody	Neuse River	Trent River	Upper Broad Creek	Goose Creek	Slocum Creek	Hancock Creek	Clubfoot Creek	Adams Creek
Number of segments	35	3	3	3	4	3	3	6
Maximum segment length (m)	7,125	2,151	1,428	1,369	2,894	2,740	1,433	2,210
Minimum segment length (m)	500	1,854	1,314	1,000	614	1,023	1,236	1,341
Maximum segment width (m)	6,739	929	1,232	760	866	728	1,295	1,578
Number of active layers	27	14	8	8	8	4	8	11

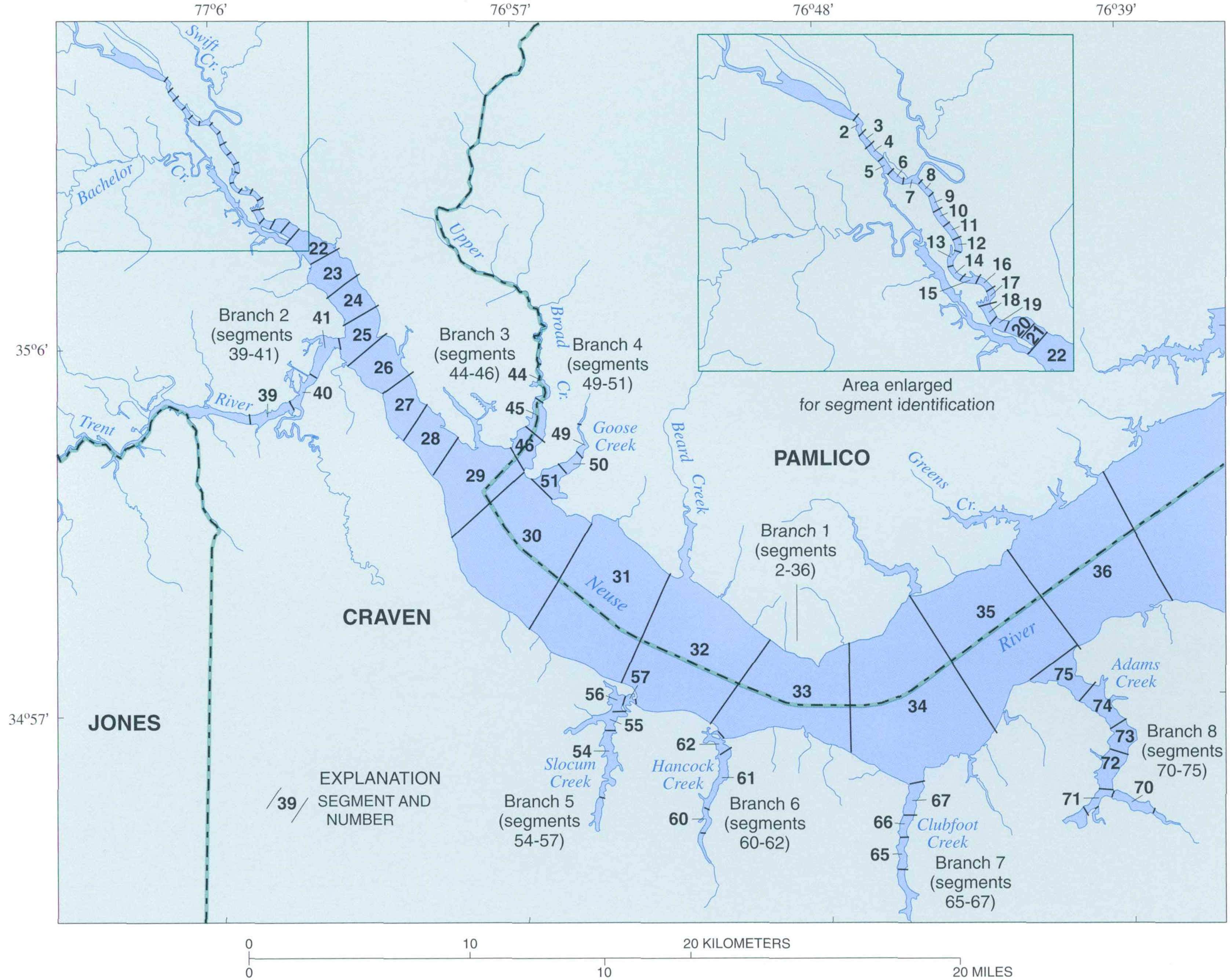


Figure 4. Modeled reach of the Neuse River estuary showing locations of branches and segments within branches.

bathymetric data are available on the Internet (National Geophysical Data Center, accessed October 7, 1998, at URL http://www.ngdc.noaa.gov/mgg/bathymetry/relief.html). Additional depth points, including data for branch 2 (Trent River), were digitized from the 1:40,000-scale chart for the Neuse River (chart number 11552). NOS data that were referenced to mean low water were adjusted to the sea level datum that was used in this model.

CE-QUAL-W2 input files were obtained for the Streets Ferry-to-New Bern water-quality model developed by Beak Consultants for Weyerhaeuser. The computational grid that was used for the Streets Ferry-to-New Bern model was transferred directly to the Neuse River estuary water-quality modeling framework and was used as obtained. Subsequent evaluations and measurements indicated that some of the bathymetry in the Streets Ferry-to-New Bern model was incorrect (Jon Mangles, North Carolina Division of Water Quality, oral commun., September 1997). In particular, depths for some of the segments between Streets Ferry and New Bern were too great, so that the number of active computational layers in branch 1 should be somewhat less than 27 (J. Bowen, The University of North Carolina at Charlotte, oral commun., April 1998).

An elevation-volume table was developed from the computational grid for the model domain (table 4). The volume obtained from the computational grid is an approximation of the actual volume, because the grid is an approximation of the actual bathymetry. The total volume of the modeled domain is 1,068 million m^3. The volume of branch 1, which extends from Streets Ferry to Oriental, is 996 million m^3. Robbins and Bales (1995) reported the volume of the reach of the estuary between New Bern and Oriental, which is part of branch 1, to be 731 million m^3.

Model Boundary Data

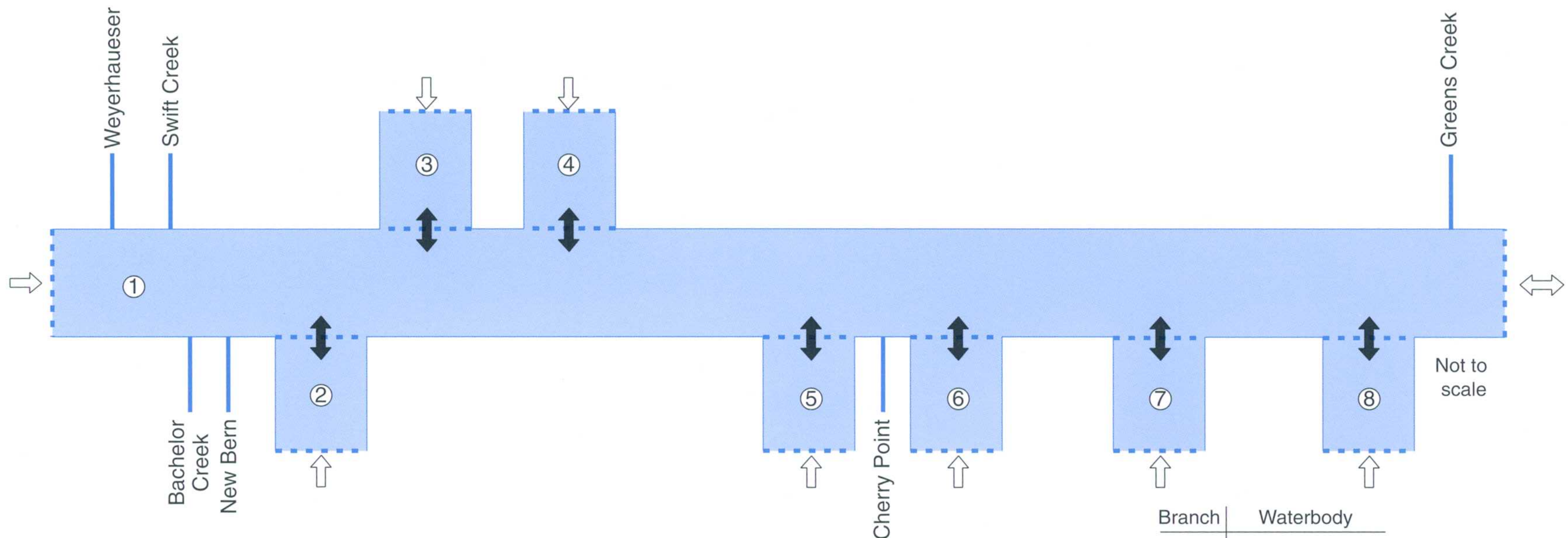
Boundaries of the Neuse River estuary water-quality model include the tributary rivers and streams, the downstream boundary at Oriental, the water surface, and the channel bottom. A time series of selected hydraulic, thermal, chemical, and other types of data are required at all model boundaries (fig. 5).

Although there has been much data collection in the Neuse River estuary during the last 10 years, it was

Table 4. Elevation-volume relation for the Neuse River estuary modeling framework computational grid

[—, not applicable]

Elevation (meters above sea level)	Volume, in million cubic meters									Number of cells
	Branch 1	Branch 2	Branch 3	Branch 4	Branch 5	Branch 6	Branch 7	Branch 8	Total	
0.25	995.96	10.26	10.62	5.28	7.82	4.14	6.28	27.88	1,068.3	806
-.25	882.43	8.15	8.41	4.07	5.57	2.67	4.75	21.78	937.8	746
-.75	768.90	5.99	6.19	2.87	3.32	1.22	3.22	15.69	807.4	686
-1.25	659.80	4.39	4.19	1.69	1.22	.26	1.84	10.49	683.9	626
-1.75	556.67	3.13	2.48	.74	.24	—	.82	6.96	571.0	566
-2.25	457.92	2.32	1.36	.30	.07	—	.28	4.24	466.5	510
-2.75	364.65	1.28	.55	.04	.05	—	.05	2.61	369.7	457
-3.25	279.60	1.33	.17	.02	.02	—	.02	1.51	282.7	408
-3.75	202.12	.96	—	—	—	—	—	.73	203.8	361
-4.25	138.22	.65	—	—	—	—	—	—	139.1	318
-4.75	86.78	.38	—	—	—	—	—	—	87.2	276
-5.25	55.04	.16	—	—	—	—	—	—	55.2	242
-5.75	32.86	.04	—	—	—	—	—	—	32.9	210
-6.25	18.43	.02	—	—	—	—	—	—	18.4	181
-6.75	9.52	—	—	—	—	—	—	—	9.52	153
-7.25	5.56	—	—	—	—	—	—	—	5.56	128
-7.75	3.06	—	—	—	—	—	—	—	3.06	103
-8.25	1.59	—	—	—	—	—	—	—	1.59	78
-8.75	.79	—	—	—	—	—	—	—	.79	55
-9.25	.29	—	—	—	—	—	—	—	.29	41
-9.75	.22	—	—	—	—	—	—	—	.22	33



Branch	Waterbody
1	*Neuse River*
2	*Trent River*
3	*Upper Broad Creek*
4	*Goose Creek*
5	*Slocum Creek*
6	*Hancock Creek*
7	*Clubfoot Creek*
8	*Adams Creek*

Boundary conditions are required at the upstream and downstream ends of all branches. Boundary conditions also are required for all tributary and point-source inflows.

EXPLANATION

- ② Branch number
- Tributary or point-source inflow (flow, salinity, temperature, water chemistry)
- Internal boundary condition, computed as part of model predictions
- Freshwater inflow boundary (flow, salinity, temperature, water chemistry)
- Saltwater inflow/outflow boundary (water level; vertical distribution of salinity, temperature, and water chemistry)
- Branch boundary

Figure 5. Modeled reach of the Neuse River estuary showing types of boundary data required at each model boundary.

difficult to identify a period when all of the data that were needed for model operation and testing were collected at the same time. After reviewing available records, the period March–October 1991 was identified as the period during which the most complete data set was collected that could be used for development of the modeling framework.

Most of the hydrologic and hydraulic data that were used to develop the modeling framework were collected by the USGS (table 5). Time series of salinity, water temperature, and DO concentrations also were collected by the USGS. Site numbers that are used in this report correspond to those used by Robbins and Bales (1995). Water-quality sampling, which included measurements of salinity, water temperature, and DO concentrations, was conducted by DWQ (previously called the Division of Environmental Management) and Dr. Hans Paerl and colleagues at The University of North Carolina Institute of Marine Sciences. However, even with all of the available data, some information that was required for model development was unavailable and had to be estimated. A description of the assumptions and data that are used to describe conditions at the model boundaries follows. Information on boundary conditions for branches and tributaries is summarized in table 6.

Table 5. Description of Neuse River estuary data-collection sites

[USGS, U.S. Geological Survey; N/A, not applicable; SR, secondary road; NC DWQ, North Carolina Division of Water Quality; UNC IMS, The University of North Carolina Institute of Marine Sciences]

Site no. (fig. 2)	Waterbody	Location	Latitude	Longitude	Measurement interval	Data source
			Streamflow			
F1	Neuse River	Kinston	35°15'29"	77°35'09"	15 minutes	USGS
F3	Trent River	Trenton	35°03'54"	77°27'24"	15 minutes	USGS
			Water level			
WL1	Neuse River	New Bern	35°06'42"	77°01'37"	15 minutes	USGS
WL3	Neuse River	Minnesott Beach	34°57'58"	76°48'20"	15 minutes	USGS
WL4	Neuse River	Oriental	35°01'26"	76°41'35"	15 minutes	USGS
			Temperature, salinity, and dissolved-oxygen concentration			
S2	Neuse River	Marker 11	34°59'56"	76°56'36"	15 minutes	USGS
S3	Neuse River	Marker 9	34°56'54"	76°48'36"	15 minutes	USGS
S4	Neuse River	Marker 1AC	34°57'24"	76°40'54"	15 minutes	USGS
S5	Neuse River	Marker 7	35°00'30"	76°39'42"	15 minutes	USGS
			Meteorology			
W1	N/A	Cherry Point Marine Corps Air Station	35°54'00"	76°53'00"	60 minutes	U.S. Navy
			Physical, chemical, and biological sampling			
Q1	Neuse River	Streets Ferry at SR 1400	35°12'30"	77°07'20"	Monthly	NC DWQ
Q2	Neuse River	Downstream from Swift Creek	35°11'25"	77°05'55"	Monthly	NC DWQ
Q3	Neuse River	Mouth of Narrows	35°09'30"	77°04'35"	Monthly	NC DWQ
WL1	Neuse River	New Bern	35°06'42"	77°01'37"	Monthly Bimonthly	NC DWQ UNC IMS
S1	Neuse River	Marker 22	35°04'48"	77°00'24"	Monthly	NC DWQ
S2	Neuse River	Marker 11	34°59'56"	76°56'36"	Monthly	NC DWQ
S3	Neuse River	Marker 9	35°56'54"	76°48'36"	Monthly	NC DWQ
S4	Neuse River	Marker 1AC	34°57'24"	76°40'54"	Bimonthly	UNC IMS
Q4	Neuse River	Mile 12 near Oriental	34°59'45"	76°41'10"	Monthly	NC DWQ
Q5	Swift Creek	NC 43 Bridge	35°13'56"	77°06'52"	Monthly	NC DWQ
F3	Trent River	Trenton	35°03'54"	77°27'24"	Monthly	NC DWQ

Table 6. Summary of boundary condition data for branches and tributaries of the Neuse River estuary

[NO_3, nitrate; NH_4, ammonium; PO_4, orthophosphorus; DO, dissolved oxygen; ppt, parts per thousand; CMD, monthly compliance monitoring data from the North Carolina Division of Water Quality. Location of sites shown in figure 2]

Waterbody	Boundary data type—Time interval of data and data source				
	Water level	Flow	Temperature	Salinity	Water chemistry (NO_3, NH_4, PO_4, DO, and biomass)
Neuse River—upstream	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Monthly; from site Q1; assumed constant for monthly reporting period; vertically uniform.
Neuse River—downstream	Hourly, site WL4	Not used	Hourly; from site S4; vertically uniform	Hourly; from site S4; vertically varying	Monthly; from site Q4; assumed constant for monthly reporting period; vertically uniform.
Trent River—upstream	Not used	Hourly; based on yields at site F3	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Monthly; from site F3; assumed constant for monthly reporting period; vertically uniform.
Upper Broad Creek—upstream	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Assumed constant and vertically uniform at minimal concentrations.
Goose Creek—upstream	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Assumed constant and vertically uniform at minimal concentrations.
Slocum Creek—upstream	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Assumed constant and vertically uniform at minimal concentrations.
Hancock Creek—upstream	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Assumed constant and vertically uniform at minimal concentrations.
Clubfoot Creek—upstream	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Assumed constant and vertically uniform at minimal concentrations.
Adams Creek—upstream	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed constant and vertically uniform at 12 ppt	Assumed constant and vertically uniform at minimal concentrations.
Weyerhaeuser discharge	Not used	CMD; assumed constant for monthly reporting period	CMD; assumed constant for monthly reporting period	Assumed zero	CMD; assumed constant for monthly reporting period; PO_4 assumed to be zero.
New Bern discharge	Not used	CMD; assumed constant for monthly reporting period	CMD; assumed constant for monthly reporting period	Assumed zero	CMD; assumed constant for monthly reporting period; PO_4 and NO_3 assumed to be zero; DO assumed to be 5.
Cherry Point discharge	Not used	CMD; assumed constant for monthly reporting period	CMD; assumed constant for monthly reporting period	Assumed zero	CMD; assumed constant for monthly reporting period; PO_4 assumed to be zero.
Swift Creek	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Monthly; from site Q5; assumed constant for monthly reporting period.
Bachelor Creek	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Assumed constant and at minimal concentrations.
Greens Creek	Not used	Hourly; based on yields at site F1	Hourly; from sites S2 and S3; vertically uniform	Assumed zero	Assumed constant and at minimal concentrations.

Streamflow

A continuous time series of either flow or water level is required at all open water boundaries. A flow boundary condition was used at the upstream end of each model branch and at each model tributary or point source (table 6). Ten tributaries to the Neuse River were included in the model domain as seven model branches, where bathymetric data were supplied for computational segments, and three model tributaries, where inputs such as inflow were supplied to individual segments. Inflows to each of these were based on hourly streamflow data that were collected at gaged locations in the lower Neuse River Basin.

Streamflow information for the lower part of the Neuse River Basin prior to 1997 was limited. As such, inflow for ungaged tributaries was supplied from a limited number of sites. Yield, or streamflow volume per time per watershed area, was computed for sites F1 and F3 for the period March 1991 through October 1991 (fig. 6A) and applied to the branches and tributaries based on drainage area at these locations

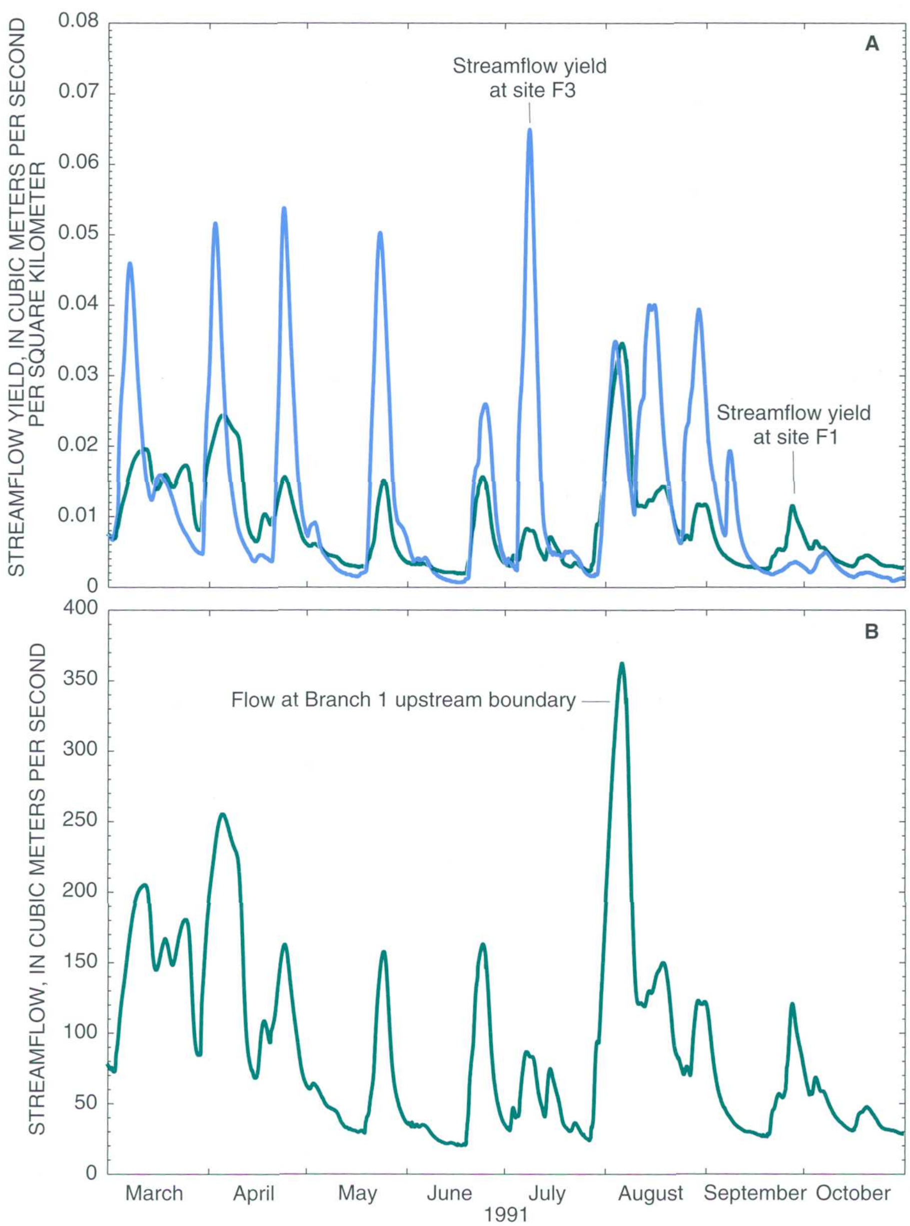


Figure 6. (A) Streamflow yields at sites F1 and F3 for March through October 1991 and (B) estimated boundary condition streamflow at Streets Ferry, N.C.

(table 7). Inflow for each model branch was obtained by multiplying drainage area at the upstream segment of each branch by hourly yield values. Yield at site F1 was applied to each branch, except the Trent River branch where yield data from site F3 were applied. Model tributary inflows for Swift Creek, Bachelor Creek, and Greens Creek also were obtained by multiplying F1 yield values by drainage area at the mouth of each of these creeks.

Table 7. Drainage areas at selected locations in the Neuse River Basin

[USGS, U.S. Geological Survey; km^2, square kilometer; SR, secondary road]

USGS station no.	Location	Drainage area (km^2)
02089500	Neuse River at Kinston (site F1, fig. 2)	7,010
02091814	Neuse River near Fort Barnwell	10,100
02091836	Neuse River at Streets Ferry	10,497
02092084	Swift Creek at mouth	869
02092092	Neuse River below Swift Creek	11,376
02092128	Bachelor Creek at mouth	166
020921620	Neuse River at New Bern (site WL1, fig. 2)	11,620
02092500	Trent River at Trenton (site F3, fig. 2)	437
02092578	Trent River at mouth	1,350
0209259275	Upper Broad Creek at mouth	143
02092626	Goose Creek at SR1100	65
02092654	Slocum Creek at mouth	135
0209265790	Hancock Creek at mouth	84
0209266300	Clubfoot Creek at mouth	60
02092669	Adams Creek at mouth	107
02092672	Greens Creek near Oriental	37
02092677	Neuse River near Oriental (site WL4, fig. 2)	14,055
02092689	Neuse River at mouth	14,547

With the exception of the mainstem branch, drainage areas applied to yield calculations for each branch and tributary were adjusted to account for unallocated drainage in the model domain. Approximately 567 km^2 of additional drainage were not specifically provided for in the measured drainage areas for the seven model branches and three model tributaries between Streets Ferry and Oriental. To adequately account for this remaining inflow, the 567 km^2 were added in the yield computation for each inflow record by a proportion relative to each tributary's contributing drainage. That is, branches and tributaries with larger drainage areas would contribute more additional flow than those with smaller drainages. For the period, March through October 1991, inflow applied at the upstream boundary ranged from 13 to 241 m^3/s with a median value of 45 m^3/s (fig. 6B).

Water Level

A continuous time series of measured water level at the downstream boundary of branch 1 was required for model operation (table 6). Data were obtained from records collected at site WL4 (fig. 2; table 5). Water-level data at site WL4 were measured with an accuracy of 0.3 cm at 15-minute intervals, and referenced to sea level (Robbins and Bales, 1995). Water-level data were supplied to the model at hourly intervals.

The North Carolina Geodetic Survey conducted a ground survey in which the datum for site WL4, as well as sites WL1 and WL3 (fig. 2; table 5), was tied to a national first-order network. Second-order vertical accuracy (for example, accuracy within plus or minus 4.2 and 5.7 cm over a 50-km survey) was achieved during the survey. However, a difference in elevation of 5 cm over a 50-km distance is approximately equal to the typical water-surface slope in the Neuse River estuary.

Water levels at site WL4 ranged from -0.320 m to 0.920 m during March through October 1991. During 1988–92, which is the entire period for which water-level data were collected at site WL4, the minimum measured water level at site WL4 was -0.463 m, and the maximum observed water level was 1.493 m (Robbins and Bales, 1995). The daily water-level range (difference between daily maximum and daily minimum water level) was 0.186 m during 1988–92 at site WL4.

Water levels generally were higher in the fall than in the spring and summer during March through October 1991 (fig. 7), which was typical during the entire data-collection period of 1988–92. However, the daily water-level range generally was greater in the spring than in the fall, with the maximum monthly mean daily range occurring in April (0.227 m) and the minimum occurring in October (0.146 m). Increased water-level fluctuations correspond to increased energy available for mixing and transport processes.

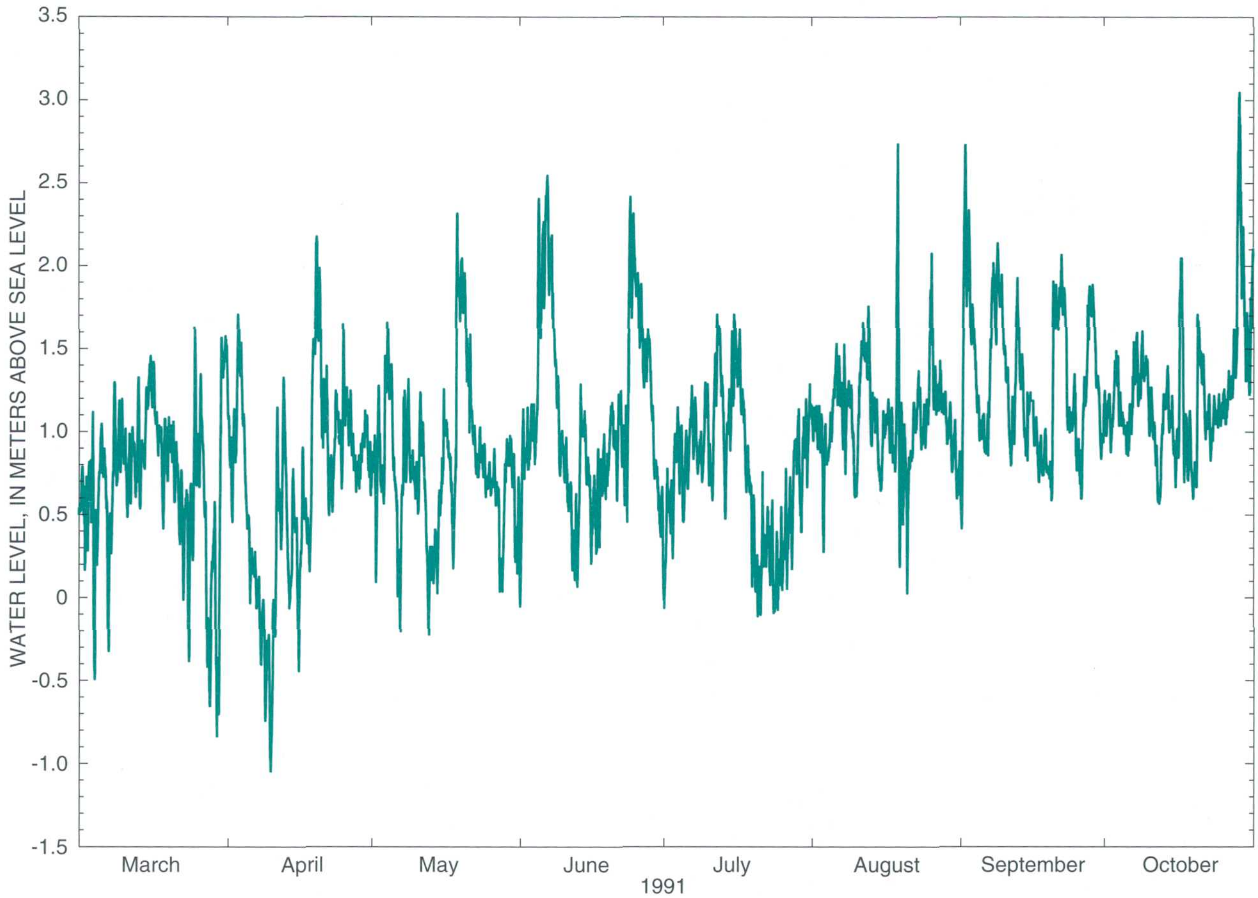


Figure 7. Water levels for March through October 1991 at Oriental, N.C. (downstream boundary condition).

Water-level data that were collected at sites WL1 and WL3 (fig. 2; table 5), located within the model domain, were available for model performance testing. Performance testing is done by comparing measured data to predicted results.

Water Temperature

Simulations of water temperature are mathematically linked to simulations of hydrodynamics. The equations that are used to predict current speed and direction include density, which is controlled by water temperature and salinity. Consequently, the density field affects current magnitude and direction and, thus, the distribution of heat and salt in the estuary. Temperature has a minor effect on density in the Neuse River estuary relative to salinity, but temperature has a major effect on water-quality simulations because of the temperature dependence of chemical reactions.

Water temperature was measured at 15-minute intervals at sites S2, S3, S4, and S5 (fig. 2; table 5). Sensors were located about 0.5 to 1.0 m below the water surface. The measurement standard range for the temperature sensor was 0 to 50 °C. Temperature measurements were accurate to within plus or minus 1 percent of full scale. Vertical profiles (0.3-m vertical intervals) of water temperature were measured when the sites were visited, which occurred at 2- to 4-week intervals. Garrett (1992) reported additional information on field techniques and data processing. Data collection at the sites continued from 1989 to 1992, and data were reported by Garrett and Bales (1991) and Garrett (1992, 1994).

A continuous time series of water temperature is required at all open-water boundaries of the water-quality model (table 6). The open-water boundaries are the upstream ends of all eight branches and the downstream end of branch 1. Water temperature data that were collected at sites S2, S3, and S4 were used to develop temperature boundary conditions. Data from sites S3 and S4 were available for model performance testing.

Data for the upstream boundary conditions were obtained from water temperature records that were collected at sites S2 and S3. Measurements at site S2 were used as the primary record. No data were available at site S2 from mid-June through July 1991. Consequently, a linear relation between measured water temperature at site S2 and measured water temperature at site S3 was developed for the period when synchronous data were available at both sites. The relation was then used to estimate water temperature at site S2 from measured temperature at site S3 for the mid-June through July period. Water temperature data were supplied to the model at hourly intervals.

This approach in developing upstream water temperature boundary conditions is based on several assumptions.

- *There is no top-to-bottom difference in water temperature at the upstream end of the eight branches.* This assumption is probably valid because (a) little or no vertical temperature gradient typically occurs in free-flowing rivers, such as at Streets Ferry, the upstream boundary of branch 1, and (b) water depths are relatively shallow at the upstream ends of branches 2–8, so it is unlikely that vertical gradients, if they existed, were significant.

- *Missing record at site S2 can be reliably predicted from records at site S3.* The relation between water temperature at sites S2 and S3 was very strong, which is not surprising because the sites are only about 15 km apart and in similar settings.

- *Water temperature at site S2 is representative of water temperature at the upstream boundaries of all eight branches.* There was no information on temperature at the upstream boundaries for comparison with measured data at site S2. It is likely that water temperatures at site S2 overestimate simultaneously occurring water temperatures at the upstream boundaries of the branches. The water likely warms at site S2, which is in the open estuary where currents are slow compared to the Neuse River at Streets Ferry and the heads of the tidal creeks, where the streams are sheltered and currents are higher. However, the general pattern of daily and seasonal temperature variations at the upstream boundaries and at site S2 is probably the same. Errors in temperature boundary conditions will have little effect on the simulation of hydrodynamics in the estuary but may affect water-quality simulations. An analysis of the sensitivity of water-quality predictions to upstream temperature boundary conditions is needed.

Data for the water temperature boundary condition at the downstream end of branch 1 generally were obtained from records collected at site S4 (fig. 2; table 5). Data were available from site S5 for only about 1 month (March) during the study period of March through October 1991. Missing data at site S4 were estimated from a relation between measurements at sites S4 and S3. The downstream boundary required a vertical distribution of water temperature. However, the water temperature was assumed to be the same from top to bottom, with all temperatures equal to the measured near-surface temperature. This assumption was made because (1) top-to-bottom water temperatures seldom differ by more than 2 °C (for example, Garrett, 1994), (2) the vertical temperature gradients are relatively unimportant for hydrodynamic and water-quality considerations, (3) the vertical distribution of water temperature within the model domain away from model boundaries is relatively insensitive to the vertical distribution at the boundary, and (4) only near-surface data were available.

Water temperature at the upstream boundaries ranged from 8.9 to 30.4 °C during March through October 1991 (fig. 8A). Water temperatures at the downstream boundary (fig. 8B) ranged from 8.9 to 32.4 °C during the same period. Near-surface water temperatures at the boundaries were between 25 and 30 °C much of the period; the mean water temperature at the downstream boundary was 24.7 °C, and the median temperature was 27.1 °C during the period. Diurnal water temperature variations were typically about 2 to 4 °C.

Salinity

Longitudinal and vertical salinity gradients exert great control on hydrodynamics and constituent transport in the Neuse River estuary. Longitudinal salinity gradients generate net upstream near-bottom flows. For example, Wells and Kim (1991) made monthly measurements of currents in a 30-km reach of the estuary upstream from site S3 (fig. 2; table 5) for 1 year. Currents in the bottom 1 m of water throughout the 30-km reach were directed upstream throughout

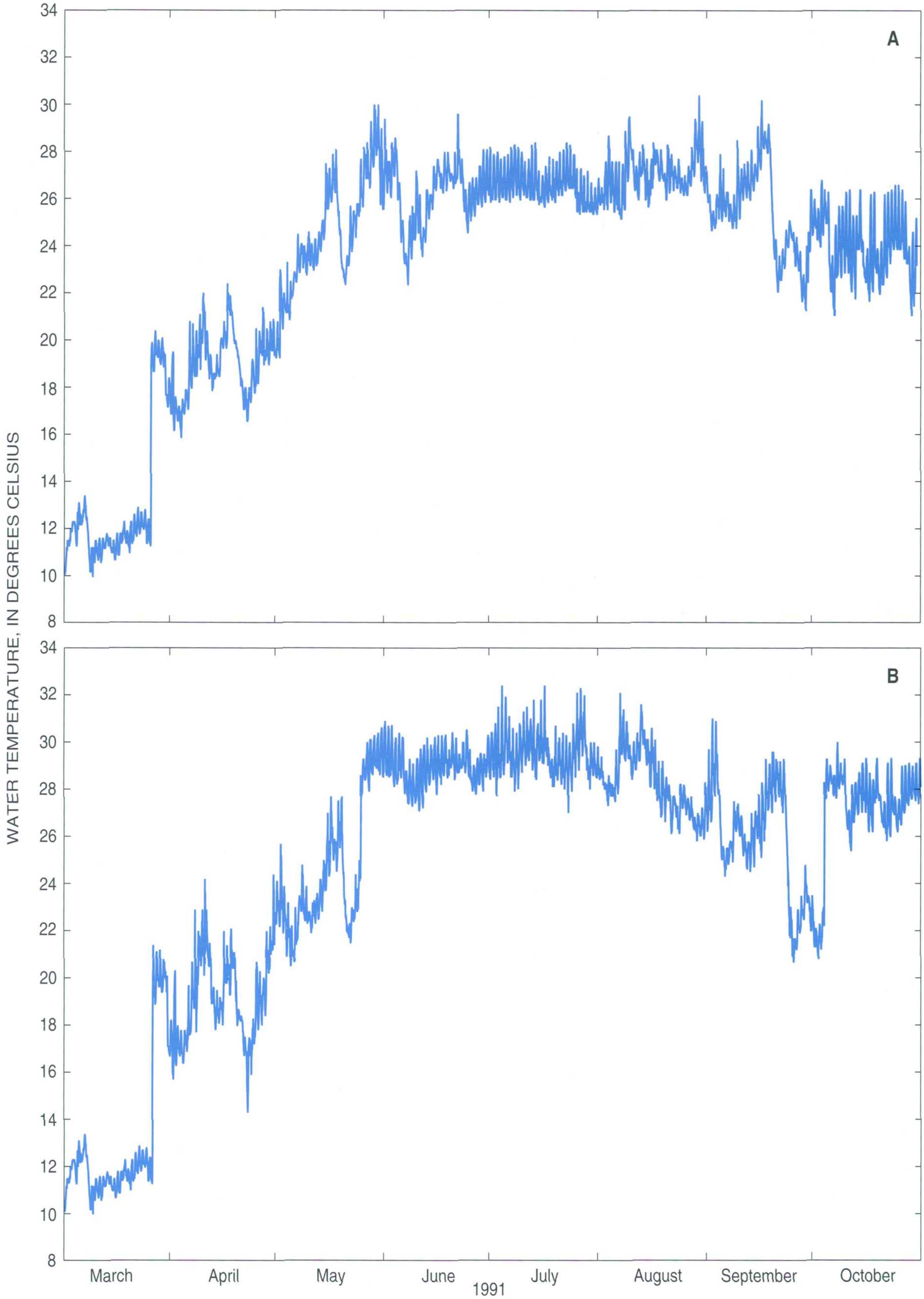


Figure 8. Water temperatures at (A) upstream boundaries of all branches and (B) downstream boundary of branch 1 for March through October 1991.

every measurement. Robbins and Bales (1995) reported that near-bottom currents measured continuously at 10 locations in the estuary and at 5-minute intervals were directed in the upstream and the downstream directions during the 17-day meter deployment.

Specific conductance was measured at 15-minute intervals at sites S2, S3, S4, and S5 (fig. 2; table 5). Sensors were located about 0.5 to 1.0 m below the water surface and about 0.5 m above the channel bottom. All measurements were referenced to 25 °C. Measurement ranges of 0 to 100; 0 to 1,000; 0 to 10,000; or 0 to 100,000 μS/cm could be selected, depending on ambient conditions. Measurements were accurate to plus or minus 3 percent of the selected full scale in a temperature range of 0 to 40 °C. Vertical profiles (0.3-m vertical intervals) of specific conductance were measured when the sites were visited, which occurred at 2- to 4-week intervals. Salinity was computed from specific conductance records by using the formulation given by Miller and others (1988). Garrett (1992) reported additional information on field techniques and data processing. Data collection at the sites continued from 1989 to 1992, and data were reported by Garrett and Bales (1991) and Garrett (1992, 1994).

As with water temperature, a continuous time series of salinity is required at all open-water boundaries of the water-quality model (table 6). Salinity at the upstream end of all eight branches, with the exception of branch 8 (Adams Creek), was assumed to be zero. Salinity data collected at site S4 (fig. 9) were used to develop the salinity boundary condition for the downstream end of branch 1. The time series of the vertical distribution at the downstream end of branch 1 was obtained by linearly interpolating between measured near-surface and near-bottom values for each time interval. Salinity data were supplied to the model at hourly intervals. Salinity at the upstream boundary of branch 8 was assumed to be constant and vertically uniform at 12 ppt. Data from sites S2 and S3 and vertical profiles of salinity were available for model performance testing.

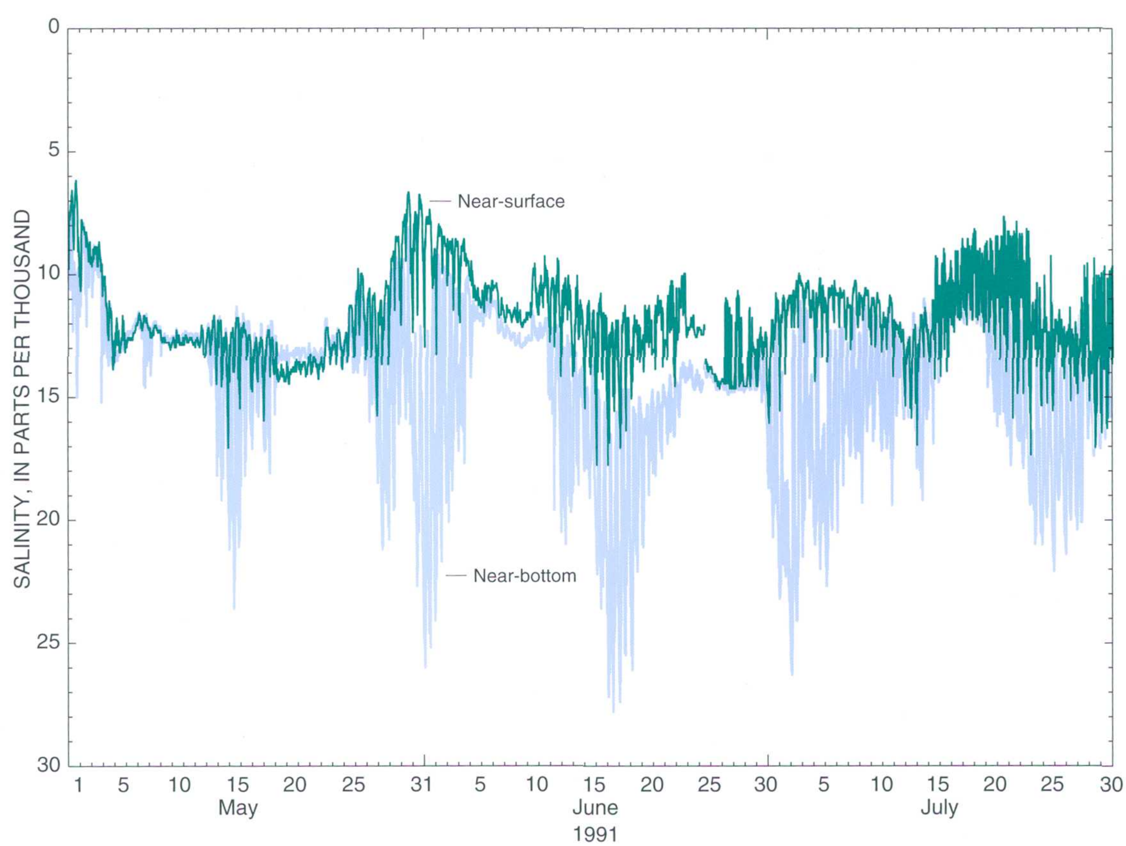


Figure 9. Near-surface and near-bottom salinity for site S4, Neuse River estuary, during May through July 1991.

During March through October 1991, near-surface salinity at site S4 ranged from 3.3 to 17.8 ppt, and near-bottom salinity ranged from 5.7 to 27.8 ppt (table 8). Although the difference between top and bottom salinity at site S4 was as much as 17.7 ppt during the period, the mean difference was 1.6 ppt, and the median difference was only 0.7 ppt. Consequently, there was little stratification at site S4 for at least half of the time during March through October 1991.

Salinity was typically much more variable at site S4, located near the mouth of Adams Creek, than at sites S2 and S3 (fig. 10). Because of the presence of the Intracoastal Waterway, Adams Creek is directly connected to the Atlantic Ocean through Beaufort Inlet. The distance from site S4 to Beaufort Inlet is about 35 km, or less than the length of the Neuse River estuary. Maximum observed salinity at site S4 was greater than that measured at a continuous monitoring station near Oriental (Robbins and Bales, 1995). Moreover, a strong tidal signal often appears to be present in salinity data from site S4 (fig. 10), but is not present in data collected at sites S2 and S3. Consequently, it appears that Adams Creek may be a source of salt to the Neuse River estuary and likely has a significant effect on the dynamics of the lower estuary.

Chemical Constituents

Water-quality samples were collected and field measurements were made at 10 sites in the study area and 1 site on the Trent River upstream from the study area by the DWQ (table 5). Samples were collected by staff from the University of North Carolina Institute of Marine Sciences (UNC IMS) at two sites in the study area (table 5). DWQ methods were documented in North Carolina Department of Environment, Health, and Natural Resources (1996); UNC IMS procedures were documented by Paerl and others (1995).

Samples were collected at monthly intervals by the DWQ and at approximately bimonthly intervals by UNC IMS. The DWQ collected water samples at the surface, whereas UNC IMS collected samples at the surface and near the bottom. Vertical profiles of water temperature, salinity, pH, and DO concentration were measured at the time water samples were collected. UNC IMS also measured light extinction at selected times when samples were collected. Samples were analyzed for a broad range of constituents, not all of which are needed for development and testing of the modeling framework.

As with water temperature and salinity, a continuous time series of water chemistry parameters is required at all open-water boundaries of the water-quality model (table 6). Concentrations of the following constituents were provided at the upstream boundaries of all eight branches: NO_3, NH_4, PO_4, biomass, and DO. Chlorophyll *a* was converted to biomass (in milligrams per liter) by multiplying chlorophyll *a* values in micrograms per liter by 0.067 (Cole and Buchak, 1995). Water chemistry data were supplied to the model at approximately monthly intervals—the measurement interval and conditions at intervening computational time steps were interpolated from the monthly data.

Data from sites Q1 and Q4 (fig. 2; table 5) were used to describe boundary conditions on the mainstem of the estuary; data from site F3 were used to estimate upstream water chemistry boundary conditions for branch 2 (Trent River); and data from site Q5 were used to estimate inputs from Swift Creek. No data were available with which to estimate upstream water chemistry boundary conditions for branches 3–8. Consequently, water chemistry was assumed to be

Table 8. Measured salinity characteristics at three sites in the Neuse River estuary during March through October 1991

[Values are parts per thousand. Difference, statistic based on individual differences between concurrently measured bottom and top salinities]

Salinity statistic	Site (fig. 2)								
	S2			S3			S4		
	Top	Bottom	Difference	Top	Bottom	Difference	Top	Bottom	Difference
Mean	4.8	10.2	5.0	8.8	10.2	1.3	11.2	12.8	1.6
Median	4.6	9.7	3.5	8.8	10.1	1.0	11.4	12.3	.7
Maximum	11.4	18.2	17.2	14.2	18.3	10.9	17.8	27.8	17.7
Minimum	.3	3.6	0	3.2	3.6	0	3.3	5.7	0
Variance	5.8	9.0	14.5	4.8	5.8	2.5	3.8	8.7	7.2

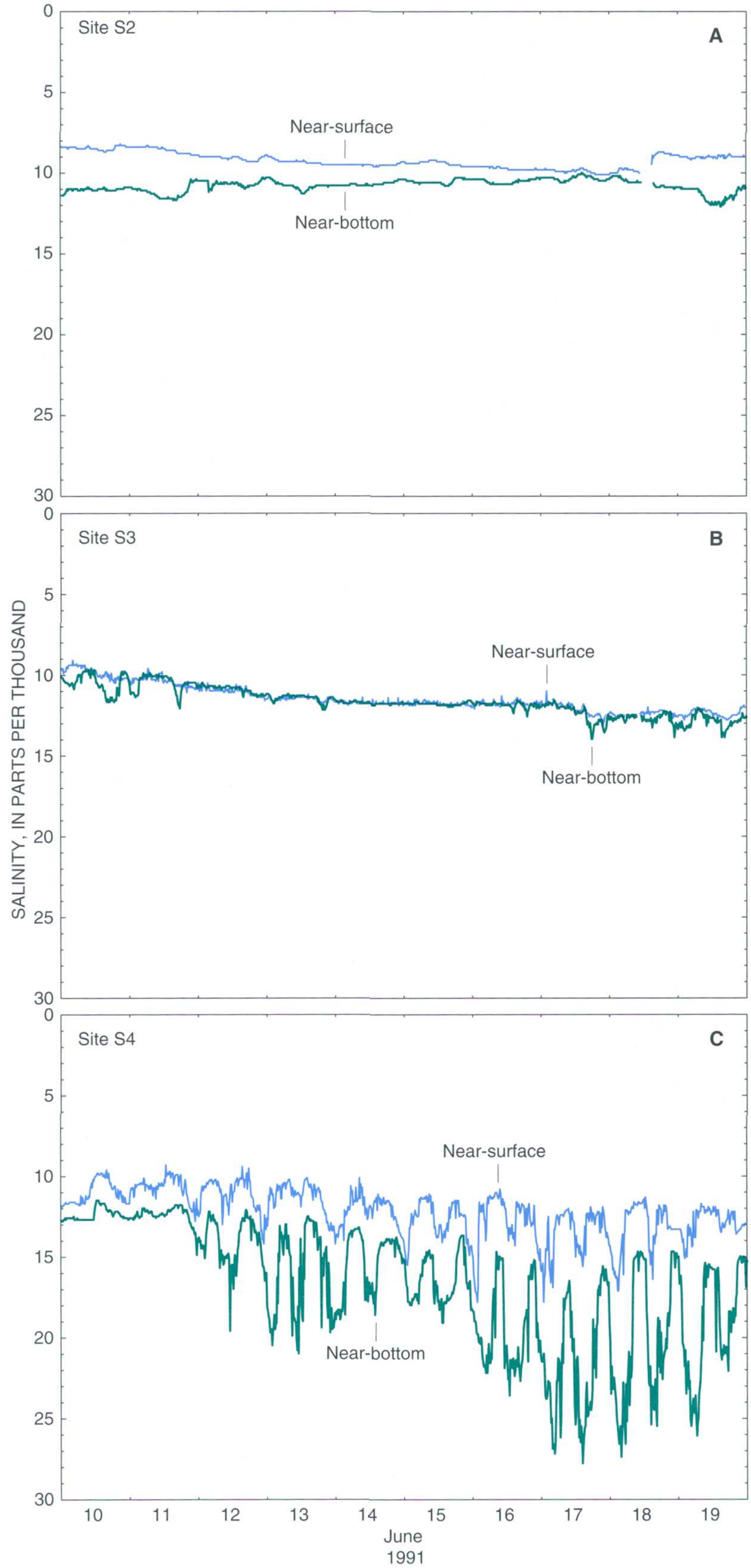


Figure 10. Plot of near-surface and near-bottom salinity for sites (A) S2, (B) S3, and (C) S4, Neuse River estuary, during June 10–19, 1991.

constant or steady, with NO_3, NH_4, and PO_4 concentrations constant at 0.01 mg/L; DO constant at 5 mg/L; and chlorophyll *a* constant at 1 μg/L.

Water chemistry was assumed to be vertically uniform at all boundaries, because only surface samples were collected at sites Q1, Q4, and F3. Concentrations of NH_4 and PO_4 are often greater near the bottom of the estuary than near the water surface because these materials are released, or regenerated, from bottom sediments under anoxic conditions. Water chemistry data from sites Q2, Q3, Q4, WL1, S1, S2, S3, S4, and S5, and vertical profiles of DO are available for model performance testing.

During March through October 1991, the mean NH_4 concentration at site WL1, located at river kilometer 13.55 (fig. 11), was about equal to that reported by Paerl and others (1995; table 1). However, the mean NO_3 concentration during March through October 1991 was somewhat greater than the longer term mean value reported by Paerl and others (1995), but the mean chlorophyll *a* concentration at WL1 was less than the longer term mean value (table 1). Flows in the Neuse River generally were lower than normal during March through October 1991, with the exception of August. Although Lebo (1995) observed that NO_3 concentrations are inversely related to flow, the higher-than-average NO_3 concentrations do not appear to be explained in this case by high inflows.

Spatial patterns in NH_4, NO_3, PO_4, and chlorophyll *a* during March through October 1991 were similar to patterns observed by Lebo (1995), Paerl and others (1995), and Pinckney and others (1997). The increase in chlorophyll *a* with distance down the estuary is consistent with patterns observed by Pinckney and others (1997) during 1994–96. Phytoplankton production or growth rates were observed to be greatest in the upper reaches of the estuary, which then translated to high biomass (chlorophyll *a*) further downstream as a result of transport processes.

Meteorology and Atmospheric Deposition

A time series of meteorological data is required for the period for which model simulations are to be made. Meteorological data are needed to help ensure that water temperature in the estuary is correctly simulated. Wind data are used in the simulation of reaeration and currents in the estuary. Required data include air temperature, dewpoint temperature, wind speed, wind direction, and a variable that describes cloud cover.

Data were obtained from the Cherry Point Marine Corps Air Station (MCAS) (site W1, table 5). Data generally were recorded by hand at hourly intervals, and copies of logs were made available to the USGS. Cherry Point is located in the downstream one-third of the study reach. Because the model does not accommodate spatially varying meteorological conditions, the assumption was made that meteorological conditions observed at Cherry Point were representative of conditions throughout the study reach.

The annual difference between evaporation from and precipitation to the Neuse River estuary is about 4 m^3/s, which is fairly small relative to the total flow in the estuary. However, the total annual volume associated with this difference represents about 20 percent of the total volume of the estuary at any given time. As a first approximation, the modeling framework does not include precipitation or evaporation in the water balance, although the heat loss associated with evaporation is included in the heat budget.

Nutrient inputs associated with atmospheric deposition have not been included in this initial modeling framework, primarily because a time series of measurements of the nutrient content of precipitation was not available. However, direct atmospheric deposition of dissolved inorganic nitrogen (NO_3 and NH_4) may be equivalent to between 2 and 200 percent of the riverine input of dissolved inorganic nitrogen to the estuary, depending on the inflow and the time of year (Paerl and others, 1995). Consequently, future monitoring and modeling activities need to include the collection of atmospheric deposition data at weekly intervals and simulation of the effects of this deposition on instream water quality.

Point Sources

The modeling framework included six point sources (figs. 4 and 5). Two types of point sources were represented in the model—(1) actual point-source discharges from wastewater-treatment facilities and (2) tributary inflows treated as a point source. Within

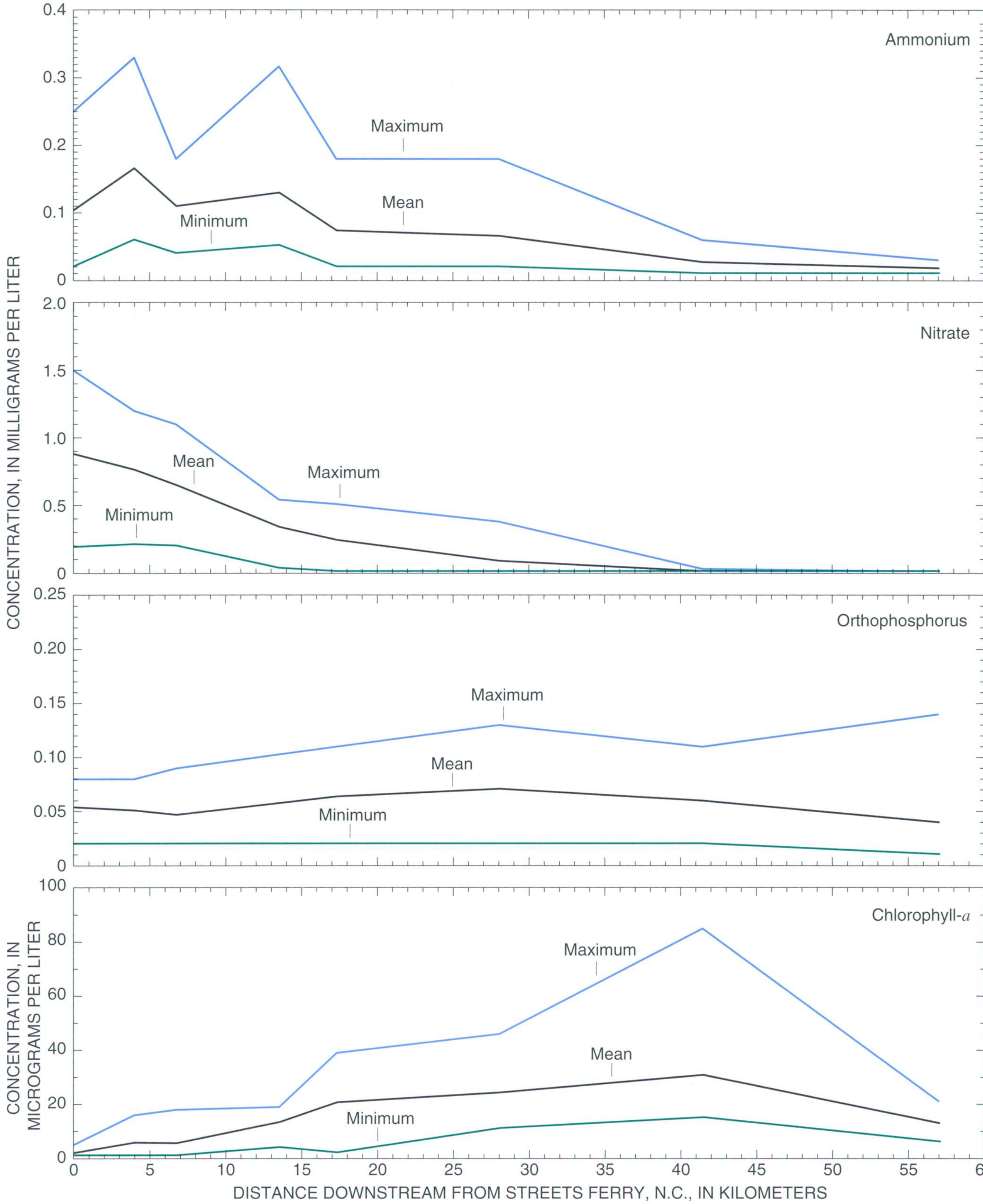


Figure 11. Maximum, mean, and minimum concentrations of (A) ammonium, (B) nitrate, (C) orthophosphorus, and (D) chlorophyll *a* in the Neuse River estuary during March through October 1991.

the model, tributary inflows contribute flow, heat, and water-quality loads to the estuary in the same way as the lateral branches (branches 2–8). However, there is no exchange between the mainstem of the estuary and the tributary inflows, unlike the lateral branches for which physical and chemical conditions are simulated. The vertical placement of a point source within the computational grid is specified as part of the model control file.

The point-source discharges from wastewater-treatment facilities were (1) Weyerhaeuser Company, (2) the City of New Bern, and (3) Cherry Point MCAS. Flow, water temperature, and water chemistry conditions (table 9) for these point sources were based on monthly compliance monitoring data obtained from the DWQ (Jon Mangles, North Carolina Division of Water Quality, written commun., August 1996). Conditions were assumed to be constant for the monthly reporting period.

Compliance monitoring data from the point sources were not available for many of the water chemistry constituents of interest, so assumptions were made about constituent concentrations in order to construct the input files for the model. PO_4 data were not available for these facilities, so PO_4 concentrations in the discharges were assumed to be zero. PO_4 loads from these facilities are likely much less than the PO_4 load from the river, but realistic PO_4 concentrations should be used when the model is calibrated and applied. PO_4 data from facilities similar to the three included in this modeling framework could be used to estimate PO_4 loads in the absence of facility-specific data. NO_3 concentrations in the New Bern discharge were assumed to be zero, and DO concentrations in the discharge were assumed to be 5 mg/L. Model input files can easily be updated if monitoring data become available.

The tributary point sources were Swift Creek, Bachelor Creek, and Greens Creek (fig. 5). Flows in these creeks were determined as previously explained and were supplied to the model at hourly intervals. The water temperature for the tributary point sources was assumed to be the same as the upstream boundary condition for the eight branches. Salinity was assumed to be zero in each of these inflows. Water chemistry conditions for Bachelor Creek and Greens Creek were treated the same as those for branches 3–8. Initial NO_3, NH_4, and PO_4 concentrations were assumed to be constant at 0.01 mg/L; DO was constant at 5 mg/L; and chlorophyll *a* was constant at 1 µg/L. Water chemistry in Swift Creek was estimated from the DWQ ambient monitoring data, which were available at monthly intervals. NH_4 ranged between 0.09 and 0.37 mg/L; NO_3 was between 0.3 and 1.2 mg/L; PO_4 was between 0.01 and 0.07 mg/L; DO was between 2.3 and 6.5 mg/L; and chlorophyll *a* was between 1 and 9 µg/L. Water chemistry conditions were assumed to be constant for the monthly reporting period.

Other Boundary Conditions

The bottom of the estuary is assumed to be an impermeable boundary so that there is no discharge of ground water to the estuary within the model domain or loss of water from the estuary to the ground-water system. Streams and estuaries in eastern North Carolina are typically discharge areas for ground water (Winner and Coble, 1996). Weaver (1998) demonstrated that segments of the Neuse River downstream from Kinston and segments of the Trent River were ground-water discharge zones. Data from Haruthunian (1997) suggested that ground-water

Table 9. Summary of inflow, water temperature, and water chemistry for point-source discharges in the Neuse River model domain during March through October 1991

[m^3/s, cubic meter per second; °C, degrees Celsius; mg/L, milligram per liter; DO, dissolved oxygen]

Parameter	Weyerhaeuser Company	City of New Bern	Cherry Point Marine Corps Air Station
Location (model segment)	4	24	32
Flow range (m^3/s)	0.43 – 1.29	0.12 – 0.16	0.08 – 0.13
Water temperature range (°C)	15.7 – 28.9	17.2 – 26.6	16.5 – 28.6
Ammonium range (mg/L)	1.4 – 3.1	4.5 – 8.3	1.1 – 8.1
Nitrate range (mg/L)	0.5 – 2.4	No data	0.5 – 6.8
DO concentration range (mg/L)	5.4 – 19.2	No data	6.2 – 8.5

discharge to the estuary was small, so it is likely that ground-water discharge represents a fairly small proportion of the total flow in the estuary. However, the effects of this discharge on water quality remain to be determined.

The bottom of the estuary is assumed to be immobile so that sediments are not resuspended by the flow. In the Neuse River estuary, fine-grained sediments typically occupy the main channel, and sands are confined to the nearshore region (Wells, 1989; Wells and Kim, 1991). The large, mobile sand bedforms that occur in alluvial streams and open seas do not exist in the Neuse River estuary, and the assumption of an immobile bottom is reasonable under most conditions. However, in many other estuaries, resuspension of organic matter during wind events has been shown to subsequently result in lowered DO concentrations in the water column. This phenomenon almost certainly occurs in the Neuse River estuary, particularly with the large amount of organic matter present in Neuse River bottom sediments.

Heat exchange between the estuary bed and the estuary is computed from the estuary bed temperature, the simulated water temperature at the bottom of the estuary, and a coefficient of sediment-water heat exchange (table 10). The estuary bed temperature and the coefficient of heat exchange are assumed to be constant in space and time. An estuary bed temperature of 15 °C was assumed for this application. Heat exchange between the bed and the water column is typically small relative to other thermal processes.

The estuary shoreline is defined as a boundary across which there is no flow. The exact position of the shoreline changes during a model simulation because of the changing water level. Changes in shoreline position occur when computational layers (fig. 3) are added or subtracted as a result of the changing water level.

Oxygen diffuses from the atmosphere into the estuary when DO concentrations in the estuary are less than saturation concentration. Likewise, when estuarine water is super-saturated with DO (for example, during algal blooms in daylight hours), oxygen diffuses from the estuary into the atmosphere. Exchange rates are governed by wind speed, water temperature, barometric pressure, and the molecular diffusivity of oxygen. Applications of CE-QUAL-W2 to Rhodhiss Lake (Giorgino and Bales, 1997) and Lake Hickory (Bales and Giorgino, 1998), both of which are located in the western Piedmont of North Carolina, indicated that reaeration rates were too small as computed by the algorithm in the model. A similar result was observed in applications of the model to the Tualatin River, Oregon (S.A. Rounds, U.S. Geological Survey, oral commun., October 1996). Consequently, the reaeration algorithm was modified for the western Piedmont reservoir applications. This modified algorithm was used in the Neuse River estuary model, as well.

Model Parameters

Parameters are used to describe physical and chemical processes not explicitly described in the governing equations, and to provide chemical kinetic rate information. Many of these parameters cannot be

Table 10. Hydraulic and thermal coefficients specified in model input

[m/s, meter per second; watts/m^2/°C, watts per square meter per degrees Celsius; m^2/s, square meter per second]

Parameter	Purpose	Value in Neuse model	Constant or time variable
Chezy coefficient	Represent turbulent exchange of energy at channel bottom	70 m$^{0.5}$/s	Constant
Sediment-water heat exchange coefficient	Compute heat exchange between channel bottom and overlying water	7 x 10^{-8} watts/m^2/°C	Constant
Wind sheltering coefficient	Reduce/increase effects of measured wind to effective speed at water surface	1.0 (dimensionless)	Time variable
Longitudinal eddy viscosity	Represent laterally averaged longitudinal turbulent transport of momentum	1 m^2/s	Constant
Longitudinal eddy diffusivity	Represent laterally averaged longitudinal turbulent transport of heat and mass	1 m^2/s	Constant

measured directly and are often adjusted during model testing until simulated results agree with observations.

Most of the relevant hydrodynamic and thermal processes are modeled in CE-QUAL-W2, so there are relatively few adjustable hydraulic and thermal model parameters (table 10). The Chezy coefficient is used to describe the extraction of energy from the mean flow by the resistance to flow caused by the channel bottom. The resistance to flow varies with the magnitude of the flow, but a single, temporally and spatially invariant Chezy coefficient value is used for the entire model domain. Model results are not sensitive to the coefficient of bottom heat exchange, but results are sensitive to the magnitude of the wind-sheltering coefficient. This coefficient is used to adjust measured wind speed to account for open-water or topographic sheltering effects. The longitudinal eddy viscosity describes horizontal turbulent exchange of momentum, and the eddy diffusivity describes horizontal mixing of mass and heat. Because of the relatively coarse computational grid, Neuse River estuary model results are somewhat sensitive to the magnitude of these values.

Fifty-seven separate parameters are used to describe physical and chemical processes simulated by the numerical model (table 11.) The values given in table 11 are based on recommendations by Cole and Buchak (1995) and on the experience of users in other applications of CE-QUAL-W2. Use of the parameters somewhat simplifies application of the water-quality model, because complex processes are described by using relatively simple relations. However, the use of 57 parameters also introduces a high degree of uncertainty in model results, because results depend on user-selected values of the parameters, and parameter selection includes a degree of professional judgment.

Most of the parameters are used to describe the effects of water temperature on chemical and biological processes. These parameters can be measured, to some extent, or estimated from field or laboratory data. As an example, algal growth does not occur at some minimum temperature and, presumably, has some optimal temperature at which growth is at a maximum. Other parameters describe the fall (settling) velocity of various constituents, which also can be measured.

The sensitivity of predicted results to model parameters was evaluated by Giorgino and Bales (1997), and Bales and Giorgino (1998) for North Carolina Piedmont lakes. For these reservoir applications, model results generally were insensitive to changes in hydraulic and thermal coefficients. Algal concentrations were sensitive to growth rate coefficient and PO_4 concentrations near the water surface, and the timing of the algal blooms was affected by the temperature rate multipliers. It is likely that Neuse River water-quality model results are most sensitive to changes in parameters controlling algal growth and decay and processes involving nitrate transformations. Results of comprehensive sensitivity testing for applications of CE-QUAL-W2 to estuaries have not been published, however. Such tests, as well as the sensitivity of model results to small changes in boundary conditions, are needed for the Neuse River estuary water-quality model.

Variable computational time steps are used in the simulations. The computational time step at each time interval is computed by a model algorithm that limits the time step in order to maintain numerical stability. The "QUICKEST" numerical scheme (Leonard, 1979) was used for solving the transport equations. A Crank-Nicholson scheme (Roache, 1982) was used to numerically solve the vertical advection equation.

Computations within the model occur at time steps substantially less than 1 hour, which is the time increment at which boundary data are available. For this application, boundary data were assumed to vary linearly between measured values.

Table 11. Physical and water chemistry parameters specified as model input

[m, meter; $(m^3/m)/g$, cubic meter per meter per gram; m/d, meter per day; d, day; DOM, dissolved organic matter; watts/m^2, watts per square meter; °C, degrees Celsius; DO, dissolved oxygen; POM, particulate organic matter (detritus); $(g/m^2)/d$, gram per square meter per day; BOD, biochemical oxygen demand; SOD, sediment oxygen demand; g/m, gram per meter; mg/L, milligram per liter]

Parameter	Computational purpose	Value in Neuse model
Light extinction coefficient for water	Amount of solar radiation absorbed by water in the surface layer.	0.45/m
Light extinction coefficient for organic solids	Amount of solar radiation absorbed by solids in surface layer.	0.2 $(m^3/m)/g$
Fraction of incident solar radiation absorbed at water surface	Amount of solar radiation absorbed at the water surface.	0.45 (dimensionless)
Suspended solids settling rate	Settling rates and sediment accumulation on the bottom of the estuary.	2 m/d
Algal growth rate	Maximum gross algal production rate, uncorrected for respiration, mortality, excretion, or settling; temperature dependent.	2/d
Algal mortality rate	Maximum algal mortality; temperature dependent.	0.1/d
Algal excretion rate	Maximum algal photorespiration rate, which becomes labile DOM.	0.04/d
Algal dark respiration rate	Maximum algal dark respiration rate.	0.04/d
Algal settling rate	Representative settling velocity for algal assemblages.	0.1 m/d
Saturation light intensity	Saturation light intensity at maximum algal photosynthesis rate.	100 watts/m^2
Fraction of algal biomass lost by mortality to detritus	Detritus and DOM concentrations; remaining biomass becomes labile DOM.	0.8 (dimensionless)
Lower temperature for algal growth	Algal growth rate as a function of temperature.	10 °C
Fraction of algal growth rate at lower temperature	Algal growth rate as a function of temperature.	0.1 (dimensionless)
Lower temperature for maximum algal growth	Algal growth rate as a function of temperature.	30 °C
Fraction of maximum growth at lower temperature	Algal growth rate as a function of temperature.	0.99 (dimensionless)
Upper temperature for maximum algal growth	Algal growth rate as a function of temperature.	35 °C
Fraction of maximum growth at upper temperature	Algal growth rate as a function of temperature.	0.99 (dimensionless)
Upper temperature for algal growth	Algal growth rate as a function of temperature.	40 °C
Fraction of algal growth at upper temperature	Algal growth rate as a function of temperature.	0.1 (dimensionless)
Labile DOM decay rate	DO loss and production of NH_4 and PO_4 from algal decay; temperature dependent.	0.3/d
Labile to refractory DOM decay rate	Transfer of labile to refractory DOM.	0.01/d
Maximum refractory DOM decay rate	DO loss and production of NH_4 and PO_4 from decay of refractory DOM; temperature dependent.	0.001/d
Detritus decay rate	DO loss and production of NH_4 and PO_4 from decay of POM.	0.08/d
Detritus settling velocity	Loss of POM to bottom sediments.	2 m/d
Lower temperature for organic matter decay	POM and DOM decay as a function of temperature.	5 °C
Fraction of organic matter decay at lower temperature	POM and DOM decay as a function of temperature.	0.1 (dimensionless)
Temperature for maximum organic matter decay	POM and DOM decay as a function of temperature.	30 °C
Fraction of maximum organic matter decay at upper temperature	POM and DOM decay as a function of temperature.	0.99 (dimensionless)
Sediment decay rate	Decay of organic matter in bed sediments.	0.08/d

Table 11. Physical and water chemistry parameters specified as model input—Continued

[m, meter; (m^3/m)/g, cubic meter per meter per gram; m/d, meter per day; d, day; DOM, dissolved organic matter; watts/m^2, watts per square meter; °C, degrees Celsius; DO, dissolved oxygen; POM, particulate organic matter (detritus); (g/m^2)/d, gram per square meter per day; BOD, biochemical oxygen demand; SOD, sediment oxygen demand; g/m, gram per meter; mg/L, milligram per liter]

Parameter	Computational purpose	Value in Neuse model
Sediment oxygen demand	Zero-order sediment oxygen demand for each computational segment.	0.4 (g/m^2)/d
5-day BOD decay rate	Effects of BOD loading on DO concentration.	0.1/d
BOD temperature rate coefficient	Adjusts 5-day BOD decay rate at 20 °C to ambient temperature.	1.047 (dimensionless)
Ratio of 5-day BOD to ultimate BOD	Effects of BOD loading on DO concentration.	1.57 (dimensionless)
Release rate of PO_4 from bottom sediments	PO_4 balance; computed as fraction of SOD.	0.015 (dimensionless)
PO_4 partitioning coefficient	Describes sorption of PO_4 on to suspended sediments.	1.2 (dimensionless)
Algal half-saturation constant for PO_4	The PO_4 concentration at which the algal uptake rate is one-half the maximum uptake rate; upper concentration at which algal growth is proportional to PO_4 concentration.	0.003 g/m
Release rate of NH_4 from bottom sediments	Nitrogen balance; computed as a fraction of SOD.	0.2 (dimensionless)
NH_4 decay rate	Rate at NH_4 is oxidized to NO_3.	0.25/d
Algal half-saturation constant for NH_4	NH_4 concentration at which algal uptake rate is one-half the maximum uptake rate.	0.001 g/m
Lower temperature for NH_4 decay	NH_4 nitrification as a function of temperature.	5 °C
Fraction of nitrification at lower temperature	NH_4 nitrification as a function of temperature.	0.1 (dimensionless)
Temperature for maximum NH_4 decay	NH_4 nitrification as a function of temperature.	20 °C
Fraction of maximum nitrification at upper temperature	NH_4 nitrification as a function of temperature.	0.99 (dimensionless)
NO_3 decay rate	Rate at which NO_3 is denitrified; temperature dependent.	0.09/d
Lower temperature for NO_3 decay	Denitrification as a function of temperature.	5 °C
Fraction of denitrification at lower temperature	Denitrification as a function of temperature.	0.1 (dimensionless)
Temperature for maximum NO_3 decay	Denitrification as a function of temperature.	20 °C
Fraction of maximum denitrification at upper temperature	Denitrification as a function of temperature.	0.99 (dimensionless)
Iron release rate from bottom sediments	Iron balance; computed as a fraction of SOD.	0.5 (dimensionless)
Iron settling velocity	Particulate iron settling velocity under oxic conditions.	2 m/d
Oxygen stoichiometric equivalent for NH_4 decay	Relates oxygen consumption to NH_4 decay.	4.57 (dimensionless)
Oxygen stoichiometric equivalent for organic matter decay	Relates oxygen consumption to decay of organic matter	1.4 (dimensionless)
Oxygen stoichiometric equivalent for dark respiration	Relates oxygen consumption to algal respiration	1.4 (dimensionless)
Oxygen stoichiometric equivalent for algal growth	Relates oxygen production to algal growth	1.4 (dimensionless)
Stoichiometric equivalent between organic matter and PO_4	Relates PO_4 release to decay of organic matter	0.011 (dimensionless)
Stoichiometric equivalent between organic matter and NH_4	Relates NH_4 release to decay of organic matter	0.08 (dimensionless)
Lower DO limit	DO concentration below which anaerobic processes, such as nitrification and sediment nutrient releases, occur.	0.2 mg/L

Summary of Major Assumptions and Capabilities

The general purpose of any numerical model of estuarine hydrodynamic and water-quality processes is to represent selected important features of the natural system. The model may be used to make management decisions or to develop and test scientific hypotheses, and each use may require a slightly different approach. Development of a numerical model includes maintaining a balance among reasonable representation of important features of the estuary, available resources, scientific understanding, and the end use of the model. All physical, chemical, and biological characteristics and processes of the estuary cannot realistically be included in a numerical model because of the constraints of time and money and because of inadequate scientific understanding of many key processes. Moreover, reasonable management decisions that are based on modeling results do not necessarily require that all processes be fully represented in a model.

The purpose of this modeling framework is to estimate the effects of changes in nutrient (nitrogen and phosphorus) loads to the Neuse River estuary on nitrogen, phosphorus, dissolved oxygen, and algal concentrations in the estuary between Streets Ferry and Oriental. A number of assumptions or simplifications were made in the development of the Neuse River estuary water-quality modeling framework. Many of the assumptions were necessary because of limited data. Other assumptions were made to maintain a reasonably simple framework. In most cases, the assumptions need to be carefully evaluated through application of the modeling framework. Key assumptions are listed below.

- Longitudinal and vertical variations in physical and chemical processes are more important than lateral variations in controlling average concentrations of nutrients, DO, and algae in the estuary. A laterally averaged modeling approach is, therefore, adequate for the purpose of the modeling framework application.
- Reasonable representation of processes in tidal creeks and embayments is necessary to adequately predict changes in the mainstem of the estuary. Therefore, physical and chemical conditions in the creeks and embayments, or branches from the mainstem, may be different in the modeling framework than conditions in the mainstem of the estuary.
- CE-QUAL-W2, a laterally averaged model code with branching capabilities, is an appropriate modeling tool for building the Neuse River estuary modeling framework. The model CE-QUAL-W2 has been widely and successfully used throughout the country and is well documented and tested. Although most of the applications of the model have been to reservoir problems, the model also has been used to address estuarine circulation and water-quality issues.
- The most important hydrologic and human inputs are represented by eight branches (Neuse River, Trent River, Upper Broad Creek, Goose Creek, Slocum Creek, Hancock Creek, Clubfoot Creek, and Adams Creek), three point-source discharges (Weyerhaeuser Company, the City of New Bern, and Cherry Point MCAS), and three tributary streams (Swift Creek, Bachelor Creek, and Greens Creek).
- The estuary and relevant processes can be reasonably represented using a fairly coarse horizontal computational grid in which cell lengths range from 500 to 7,125 m, cell top widths range from 102 m to 6,739 m, and cell heights are constant at 0.5 m. Greater spatial resolution (shorter cell lengths) is appropriate in the upstream reaches of the estuary where many of the algal blooms are known to occur.
- Velocity, water temperature, salinity, and constituent concentrations are uniform within any particular computational cell.
- Available 1991 data are adequate for constructing and testing the Neuse River estuary water-quality modeling framework.
- Streamflow yields measured at site F1 (Neuse River at Kinston) adequately represent flows at all branches and tributaries, other than the Trent River, which is adequately represented by measured yields at site F3 (Trent River at Trenton).
- Near-surface water temperature measured at site S2 is representative of water temperature at the upstream boundaries of all eight branches and all three stream tributaries, with missing record at site S2 reliably predicted from records at site S3. In addition, there is no top-to-bottom difference in

water temperature at the upstream end of the eight branches.

- The salinity for the inflow to each branch of the modeling framework, except Adams Creek (branch 8), is always zero. This assumption was necessary because of the absence of data on inflow salinity. As previously discussed, Adams Creek may be a source of salinity to the Neuse River estuary, and the salinity in the Adams Creek inflow was assumed to be constant at 12 ppt.
- The vertical distribution of salinity at Oriental, the downstream end of the model, can be represented by a linear interpolation between measured near-surface and near-bottom salinity at site S5.
- Key water chemistry processes are adequately described by relations among water temperature, nitrogen (as NH_4 and NO_3), phosphorus (as PO_4), DO, organic matter decay, and algal processes (growth, photosynthesis, respiration, and mortality).
- Algae can be represented by a single phytoplankton assemblage. This means that nitrogen fixing blue-green algae are not specifically included in the model formulation, and there is no accounting for this potential source of nitrogen to the estuary.
- Monthly to bimonthly measurements of water-quality conditions (nutrient, DO, and algal concentrations) can be used to adequately represent hourly water-quality variations at all model boundaries (inflows and mainstem downstream boundary), three point-source discharges, and one tributary stream. Hourly values can be obtained by linear interpolation between measured values.
- In the absence of data, constituent loads from selected sources can be assumed to be minimal.
- The top-to-bottom difference in water chemistry at all boundaries is negligible.
- Ground-water inflow to or outflow from the estuary is insignificant.
- Meteorological conditions are spatially uniform over the entire estuary.
- Atmospheric inputs can be neglected.
- The resuspension or mixing of bottom sediments has no effect on water quality.
- PO_4 and NH_4 releases from bottom sediments can be adequately described by simple first-order reactions that are spatially uniform.
- Vertical accelerations of mass are small, and the hydrostatic pressure distribution is applicable.
- Material entering the estuary from lateral branches, point sources, or tributaries is instantaneously mixed across the estuary and along the segment into which the material is introduced.
- Mixing coefficients for mass and momentum adequately represent subgrid-scale processes. Mixing coefficients and the resistance coefficient are spatially and temporally invariant.
- Physical and water chemistry rate parameters are spatially constant.

These assumptions define the limitations of the modeling framework. However, despite these limitations, the modeling framework can be used to evaluate the effects of changes in external loadings on NO_3, NH_4, PO_4, DO, and biomass concentrations in the Neuse River estuary once it has been adequately calibrated. In addition, the model can be used to describe the movement of water, salt, and conservative materials in the estuary, as well as to describe the exchange of material between the mainstem of the estuary and embayments. A description of the relative effects of a change on estuarine conditions is a more appropriate application of the modeling framework than a focus on predictions of absolute concentrations of a substance at any particular location. The assumptions listed above also can be used to identify future research and data-collection needs in the Neuse River estuary.

SUMMARY AND SUGGESTIONS FOR MODEL REFINEMENTS

Primarily as a result of fish kills in the Neuse River estuary in 1995, nutrient reduction strategies were developed for point and nonpoint sources in the basin. However, the effects of these strategies are difficult to assess directly because of the confounding influences of weather, hydrology, diverse sources of nutrient inputs to the estuary, and complex hydrologic nutrient interactions. Because of the interannual variability in the natural system and the resulting complex hydrologic-nutrient interactions, it is difficult to detect through a short-term observational program the effects of management activities on Neuse River estuary water quality and aquatic health. However, a properly constructed water-quality model can be used to evaluate some of the potential effects of management actions on estuarine water quality. Such a model can be used to predict estuarine response to present and proposed nutrient strategies under the same set of meteorological and hydrologic conditions, thus removing the vagaries of weather and streamflow from the analysis.

A two-dimensional, laterally averaged hydrodynamic and water-quality modeling framework was developed for the Neuse River estuary by using previously collected data. However, all required data were not available to develop the model, and some information was estimated from available data. Nevertheless, the study objective, which was to develop a modeling framework that could be enhanced by using a more complete data set, was met.

Development of the modeling framework consisted of (1) computational grid development, (2) assembly of data for model boundary conditions and model testing, (3) selection of initial values of model parameters, and (4) limited model testing.

The model domain extends from Streets Ferry to Oriental, includes the mainstem of the estuary and seven lateral embayments that have continual exchange with the mainstem, three point-source discharges, and three tributary streams. There are 35 computational segments along the mainstem of the estuary, and a total of 60 computational segments in the entire framework. Each computational cell is 0.5 m thick; segment lengths range from 500 to 7,125 m.

Data that were used to develop the modeling framework were collected during March through October 1991 and represent the most comprehensive data set available prior to 1997. Most of the data were collected by the North Carolina Division of Water Quality, the University of North Carolina Institute of Marine Sciences, and the U.S. Geological Survey.

Several activities could be undertaken to build on the modeling framework described in this report. In fact, the previously described Water Resources Research Institute team is implementing many of the suggestions listed below. Most of the suggestions focus on either collection of additional data or model testing. The suggestions are listed in no particular order. Some suggestions can be implemented easily, while others will require a long-term effort.

- Collect a complete set of boundary data, including inflow rates, water temperature, salinity, and temporally detailed (at least weekly) water chemistry, at the upstream boundary of all eight branches, the three tributary streams, and the three point sources. Data other than water chemistry should be collected at 15-minute intervals.
- Collect a complete set of boundary data, including water level and vertical distributions of water temperature, salinity, and temporally detailed (at least weekly) water chemistry, at the downstream boundary of branch 1. Data other than water chemistry should be collected at 15-minute intervals.
- Obtain compliance monitoring data at more frequent (weekly to daily) intervals.
- In addition to the data described, synchronously measure conditions within the estuary, as well as meteorological conditions, to provide a complete data set for calibration and testing.
- Measure atmospheric inputs to the estuary at weekly intervals and in at least three locations.
- Develop and test a sediment sub-model that can be used to reliably predict spatially and temporally varying nutrient inputs to the estuary from bottom sediments.
- Determine the magnitude of ground-water inputs to the estuary.
- Develop the capability to simulate more than one phytoplankton assemblage so that algal succession in the estuary can be predicted.
- Determine the effect of resuspended organic material on DO concentrations in the estuary.
- Test the sensitivity of model results to refinements in the computational grid.
- Conduct field or laboratory experiments to quantify as many model parameters as possible.
- Test the sensitivity of predicted results to changes in model parameters and boundary conditions, particularly changes in the downstream water chemistry boundary.

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