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Technical Guidance Manual For Performing Waste Load Allocations
Book III: Estuaries

Part 4
Critical Review Of Coastal Embayment And Estuarine Waste Load Allocation Modeling

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TECHNICAL GUIDANCE MANUAL FOR PERFORMING WASTE LOAD ALLOCATIONS

BOOK III: ESTUARIES

PART 4: Critical Review of Coastal Embayment and Estuarine Waste Load Allocation Modeling

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Preface

The document is the third of a series of manuals providing information and guidance for the preparation of waste load allocations. The first documents provided general guidance for performing waste load allocations (Book I), as well as guidance specifically directed toward streams and rivers (Book II). This document provides technical information and guidance for the preparation of waste load allocations in estuaries. The document is divided into four parts:

Part 1 of this document provides technical information and policy guidance for the preparation of estuarine waste load allocations. It summarizes the important water quality problems, estuarine characterisitics and processes affecting those problems, and the simulation models available for addressing these problems. Part 2 provides a guide to monitoring and model calibration and testing, and a case study tutorial on simulation of waste load allocation problems in simplified estuarine systems. Part 3 summarizes initial dilution and mixing zone processes, available models, and their application in waste load allocation.

This part, "Part 4: Critical Review of Coastal Embayment and Estuarine Waste Load Allocation Modeling," summarizes several historical case studies, with critical review by noted experts. The reader should refer to the preceding parts for information on model processes, available models, and guidance to monitoring and calibration.

The technical guidance is comprehensive and state-of-the-art. Case studies of applications serve as the best teacher of the proper and improper use of this technical guidance. Similar models are often used in large freshwater coastal embayments and estuaries because there are some similarities in their hydrodynamic transport processes.Therefore, included in this part are one freshwater embayment study and three estuarine studies where models were used for waste load allocation. These studies have been selected to provide a range of representative geographic areas, freshwater bays and embayments, estuaries, and models. The studies were **not selected because they were exemplary** but rather because they represented applications of diverse approaches.

Each of the studies has particular **merits** and **deficiencies**; the balance is different in each study. Perfect examples are not always the best teachers. By examing the strengths and weaknesses of each application the reader can appreciate how to best use the technical guidance and how to avoid misuse and common problems.

The examples are summarized with only limited commentary. The information for each is presented with sufficient detail to allow the reader to understand what was done and to highlight certain noteworthy aspects. Following the case examples, three experts critique the relative merits and deficiencies in each case study and provide their opinions on the proper approach to estuarine modeling.

A draft version of this document received scientific peer review from the following modeling experts:

Steven C. Chapra,
University of Colorado-Boulder

Donald R.F. Harleman,
Massachusetts Institute of Technology

Gerald T. Orlob,
University of California-Davis

Robert V. Thomann,
Manhattan College

Their comments have been incorporated into the final version.

Organization: "Technical Guidance Manual for Performing Waste Load Allocations. Book III: Estuaries"

Part	Title
1	Estuaries and Waste Load Allocation Models
2	Application of Estuarine Waste Load Allocation Models
3	Use of Mixing Zone Models in Estuarine Waste Load Allocation Modeling
4	Critical Review of Coastal Embayment and Estuarine Waste Load Allocation Modeling

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

JUL 20 1992

OFFICE OF
WATER

MEMORANDUM

SUBJECT: Final Technical Guidance Manual For Performing Wasteload Allocations: Book III, Estuaries, Parts 3 and 4

FROM: Tudor T. Davies, Director
Office of Science and Technology (WH-551)

TO: Regional Water Management Division Directors
Regional Environmental Services Division Directors
Regional TMDL/WLA Coordinators

Attached, for national use, is the final version of the Technical Guidance Manuals for Performing Wasteload Allocations: Book III, Estuaries, Parts 3 and 4. Parts 1 and 2 were finalized during FY 91 and have been in distribution ever since for national use. We are sending extra copies of Parts 3 and 4 of the guidance document to the TMDL/WLA coordinators for distribution to the States to use in conducting wasteload allocations.

An earlier draft of Parts 3 and 4 were reviewed by your staff and their comments were considered in finalizing this guidance. Major modifications to the earlier draft include:

- The discussion on mixing zone criteria in Part 3 (see page 7-3) is now consistent with the March 1991 version of the Technical Support Document for Water Quality-based Toxics Control.

- The title of Part 4 has been modified from Critical Review of Estuarine Wasteload Allocation Modeling to Critical Review of Coastal Embayment and Estuarine Wasteload Allocation Modeling. This change was necessary because the Saginaw Bay example in Part 4 of this guidance does not meet the strict regulatory definition of an estuary.

If you have any questions or comments or desire additional information, please contact Russell S. Kinerson, Exposure Assessment Branch, Standards and Applied Science Division (WH-585), Telephone (202) 260-1330.

Attachments

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This document represents the efforts of several people and the integration of several documents. Site selection and national expert review were managed by Hiranmay Biswas, U.S. EPA Office of Science and Technology (formerly Monitoring and Data Support Division). Chapter 12 on the Manasquan along with portions of Chapter 11 were excerpted from an earlier draft Technical Guidance Manual prepared by Richard Wagner, Jane Metcalfe, and Elizabeth Southerland of JRB Associates. Chapter 10 on Saginaw Bay was prepared by Bruce Monson, Chapter 11 by David Dilks, and Chapter 13 by Paul Freedman, all of Limno-Tech, Inc. Scott Hinz and Susan Johnson of Limno-Tech are acknowledged for their work in editing this draft document.

National expert peer review of this manual was provided by Robert V. Thomann, Manhattan College, Donald R.F. Harleman, Massachusetts Institute of Technology, and Steven C. Chapra, University of Colorado at Boulder.

In addition, helpful internal review comments were received from Thomas Barnwell, U.S. EPA Athens Environmental Reasearch Laboratory; James Martin, ASci Corporation; Rick Brandes, U.S. EPA Office of Wastewater Enforcement and Compliance; Steve Glomb, U.S. EPA Office of Wetlands, Oceans, and Watersheds; Dale Bryson, U.S. EPA Region V; Mimi Dannel, U.S. EPA Region VI; Aaron Setran, U.S. EPA Region IX; Clyde Bohmfalk, Texas Water Commission, Michael Waldon, The University of Southern Louisiana; and June Harrigan, State of Hawaii. A significant part of this internal review process was managed by Karen Gourdine, U.S. EPA Office of Science and Technology.

Bruce Monson of Limno-Tech was responsible for the draft formatting of this document, and the final layout was done by Tad Slawecki, also of Limno-Tech.

10. Great Lakes Embayment Seasonal Phytoplankton Model of Saginaw Bay

10.1. Background

The Saginaw Bay is not an estuary. However, its hydrodynamic processes are similar to those observed in some shallow estuaries with wind-driven circulation. The Saginaw Bay phytoplankton model of Bierman and Dolan (1986a,b) is presented here to illustrate the application of a dynamic and kinetically complex box model to a Great Lakes embayment. This model was calibrated with two comprehensive data sets. Following significant reductions in loadings and changes in the Bay's water quality, the model projections were tested and validated (post-audit) with another comprehensive data set. The model was developed as part of a long-term study of eutrophication in Saginaw Bay. It was designed as a management and research tool to estimate phytoplankton response to various phosphorus control strategies. The model was used extensively by the USEPA and International Joint Commission to evaluate nutrient loading reductions for Saginaw Bay.

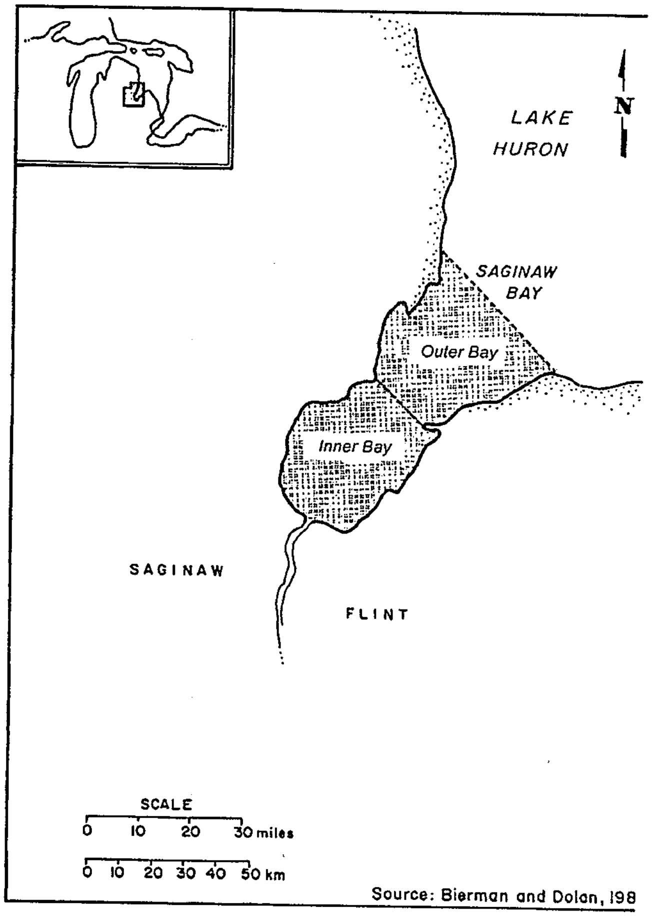

Figure 10-1. Saginaw Bay site map [Bierman and Dolan (1986a). Reprinted from ASCE Journal of Environmental Engineering, Vol. 112, No. 2. p. 401. With permission].

The authors describe the model as "a deterministic, spatially segmented, multi-class phytoplankton model." The phytoplankton comprise five functional groups: diatoms, greens, non-nitrogen-fixing blue-greens, nitrogen-fixing blue-greens, and "others." Nutrient uptake is considered for phosphorus, nitrogen, and silica. Herbivory, settling, and decomposition are mechanisms of phytoplankton depletion.

10.2. Problem Setting

Located on the western shore of Lake Huron (Figure 10-1), the Saginaw Bay watershed is approximately 21,000 km^2 (8108 mi^2). It is dominated by agriculture, forest, and four urban-industrial centers: Bay City, Flint, Midland, and Saginaw. The 1980 population for the area was slightly over 1,200,000. The area is drained by the Bay's major tributary, the Saginaw River. The River accounts for 90 percent of the tributary inflow to the Bay.

Saginaw Bay extends 90 km from the River's mouth to the Bay's opening to Lake Huron. It is broad (42 km), shallow (10 m average depth), and vertically well-mixed. The average hydraulic residence time is approximately four months.

The Bay has been characterized as behaving like a simple estuary (Ayers et al, 1956). Like estuaries, it is a nutrient-rich arm of a larger nutrient-poor water body, Lake Huron (Richardson, 1974). Furthermore, water levels and flow directions of the Bay change. Unlike an estuary, the water level is influenced by wind patterns rather than tides. Northern gales can create a seiche in the Bay that raises the water level at the mouth of the Saginaw River by more than a meter (Fish and Wildlife Service, 1956; cited by Richardson, 1974).

The International Joint Commission identified Saginaw Bay as one of forty-two Great Lakes Areas of Concern needing remedial action. Eutrophication of the Bay had caused taste, odor, and filter-clogging problems for municipal water supplies. Waste discharges and runoff have been major contributors to water quality degradation. In the late 1970's, phosphorus reduction programs were implemented at wastewater treatment plants and resulted in large reductions of phosphorus loading to the Bay. From 1975 to 1980 the phosphorus loads were reduced over 65 percent. The model was calibrated and verified when the phosphorus loadings were high (1974 and 1975) and tested in a post-audit following the large reductions of phosphorus (1980).

10.3. Model Application

Although this model's development began in a more simple form, it is presented here in its most advanced form as a spatially segmented, temporally dynamic model. A more spatially simplified precursor model (Bierman and Dolan, 1980) provided some valuable conclusions about the biological and chemical processes in the waterbody. These findings were used to develop the kinetic structure and calibrate the more spatially detailed model. For example, the factors influencing phytoplankton dynamics in the model are temperature, light, nutrients, and zooplankton grazing. Temperature and light were generally more growth-rate limiting than nutrients. However, nutrient limitation became important for peak phytoplankton crops. In the spring and fall, the primary source of phosphorus was external loading, which fed the dominant diatom crops. In mid-summer, the primary source of phosphorus was recycling within the water column and from sediments, which fed the summer blue-green crops.

The multi-class phytoplankton model was developed to predict the response of the Saginaw Bay phytoplankton to various phosphorus control strategies. Of primary concern were the nuisance, bloom-forming blue-greens that cause taste and odor problems. The emphasis in the model was on nutrient cycling since it is a limiting and controllable factor in phytoplankton growth. Several hypothetical scenarios and a post-audit are presented below following examination of the calibration and validation of the model.

10.3.1. Model Description

The model developed for Saginaw Bay falls into a general class of models called "box models." The approach involves dividing the water body into several cells (or boxes), each of which is considered completely mixed (Figure 10-2). Transport of chemicals, biomass, and water between cells occurs through advective transport and dispersion.*

The mass of pollutants, algae or other constituents in each cell changes in response to loadings, transport, mixing, settling, and reaction kinetics. A mass balance equation is written for each cell and the resulting differential equation solved simultaneously through time for all cells by a numerical method.

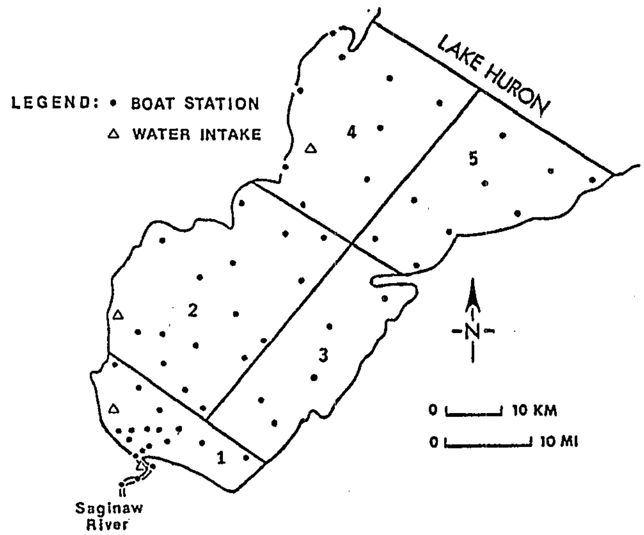

Figure 10-2. Model segmentation of Saginaw Bay [Bierman and Dolan (1986a). Reprinted from ASCE Journal of Environmental Engineering, Vol. 112, No. 2. p. 402. With permission].

The model incorporates three nutrients — nitrogen, phosphorus, and silica — each with biologically available and unavailable components, and a biomass component. It includes five classes of algae and two classes of zooplankton. The interaction of the components are shown in Figure 10-3.

The model is structured in a format to simulate a specified number of phytoplankton and zooplankton classes. The model developers chose to use multiple classes of phytoplankton and zooplankton to predict the desired decline in blue-green algae. Phytoplankton groups respond differently to zooplankton grazing and have different nutrient requirements. Unlike the many eutrophication models that use chlorophyll *a* as a surrogate for phytoplankton, this model uses phytoplankton cell biomass.

A number of mechanisms are considered in this model, including:

- Internal nutrient pool kinetics for phosphorus, nitrogen, and silicon.
- A reaction-diffusion mechanism for carrier-mediated uptake of phosphorus and nitrogen that includes luxury uptake of nutrients.

* Advective transport is defined as a flow based on system hydrodynamics (modeled or measured). Dispersion transports mass from areas of high concentration to areas of low concentration with no net flow of water.

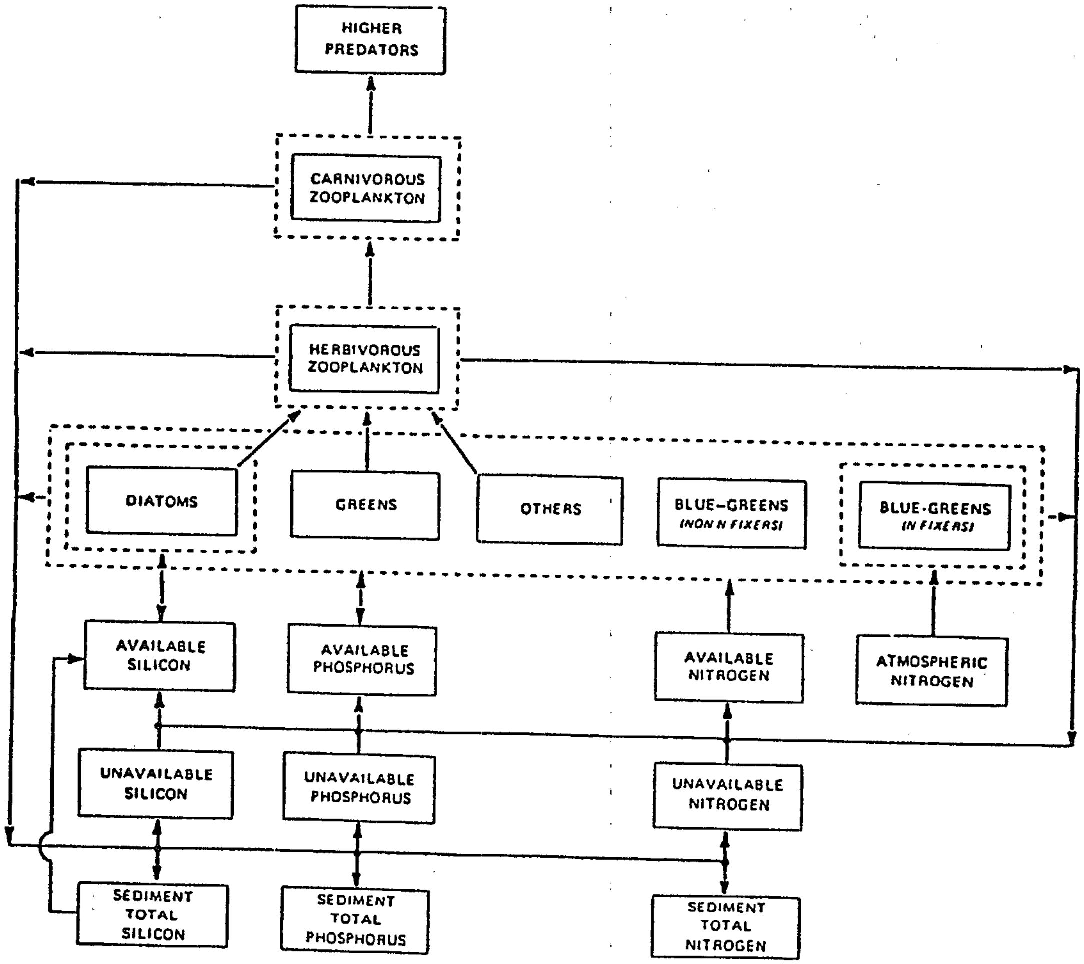

Figure 10-3. Schematic diagram of principal model compartments and interaction pathways [Bierman and Dolan (1986a). Reprinted from ASCE Journal of Environmental Engineering, Vol. 112, No. 2. p. 403. With permission].

- Biological-chemical kinetics, included in sediment compartments for total concentrations of phosphorus, nitrogen, and silicon.
- Zooplankton grazing.
- Saturation kinetics for water column nutrient mineralization.
- Saturation kinetics for phytoplankton decomposition.
- An advective-dispersive model for transport of chloride used to determine water exchange among the segments.
- Wind-dependent resuspension for sediment nutrients.

The internal nutrient pool kinetics are a noteworthy aspect of the model because they treat cell growth as a two-step process: 1) uptake of nutrients and 2) biomass growth. The common approach is a one step use of the Monod (Michaelis-Menten) equation, where cell growth is a direct function of external nutrient concentrations. The internal pool kinetics allow for accumulation of surplus internal nutrients when external nutrient concentration is high and use of internal stores when external nutrient concentration is low. The recycling of nutrients is a function of the phytoplankton losses. This more realistic approach requires greater model complexity and additional model coefficients. Furthermore, it exacts a severe computational burden because all cell history must be tracked to follow exposure patterns.

While phytoplankton growth is a function of nutrient kinetics, phytoplankton loss mechanisms include respiration, decomposition, sinking, and zooplankton grazing. Respiration loss is a temperature-dependent, first-order decay term. Microbial decomposition is a temperature-dependent, second-order decay term proportional to total phytoplankton concentration and specific growth rate. Sinking loss is set at a constant velocity for each phytoplankton class. Zooplankton grazing loss is a temperature-dependent, two-component loss mechanism. It was included for diatoms, greens, and "other" phytoplankton, but not for blue-greens. The zooplankton response function included losses to higher-order predators. A constant "refuge concentration" is specified for both phytoplankton and zooplankton below which there is no grazing or predation.

10.3.2. Model Inputs

The complexity of the model required many parameters and boundary conditions. Model coefficients are defined in Table 10-1 and values summarized in Table 10-2 (a-c) to provide the reader a sense of the model complexity.

Each phytoplankton group was characterized by a maximum growth rate, a temperature growth adjustment factor, and a saturation light intensity. Other phytoplankton coefficients included respiration rate, decomposition rate, sinking rate, and conversion rates of nutrient forms (from unavailable to available).

Zooplankton kinetic coefficients, taken from literature or data collected for this study, included assimilation efficiency, maximum ingestion rate, and phytoplankton preference factor. Growth and death rates were estimated or calibrated to field data. Coefficients were assigned for each of the two functional groups of zooplankton: fast ingesters and slow ingesters.

Nutrient uptake and cell growth were treated in the model as separate processes, but have parallel sets of equations and coefficients. Nutrient kinetics for phosphorus and nitrogen depended on the variables of percent dry weight and minimum cell quotas for these nutrients. Minimum concentrations were also assigned for external nutrients, which corresponded to the minimum levels to which the phytoplankton could deplete the environment. External and internal half-saturation levels were specified for both processes. The latter were set equal to the minimum cell quotas. Maximum phosphorus and nitrogen uptake rates were the same for all phytoplankton groups. Silica coefficients were specified only for diatoms.

Another important assumption of the model was the partitioning of phosphorus into available and unavailable components. Dissolved ortho-phosphorus was considered to be available for immediate uptake by phytoplankton. Unavailable phosphorus was equivalent to total phosphorus minus dissolved orthophosphorus. For scenarios discussed below, available and unavailable phosphorus ratios were estimated for point and nonpoint sources. The effective ratio of available to total phosphorus for point sources at the Saginaw River mouth was assumed to be 34 percent. It was also assumed that the ratio did not change with different treatment levels.

Environmental forcing functions varied for each year and included water temperature, incident solar radiation, pollutant and tributary loadings, boundary conditions, and water transport rates. They were determined independently of the model and supplied as input. Table 10-3 is a summary of selected examples of these inputs designed to provide the reader a sense of the range of values. These environmental factors were supplied to the model as time series input. Water transport rates were obtained from a separate time-variable model of a conservative tracer, chloride [Richardson (1974)].

10.3.3. Calibration/Verification

The approach to calibration was to match general trends of the seasonal changes in the data and obtain model output within one standard deviation of the mean value of the observed data for each cruise. When this was not achieved, model coefficients were adjusted to best approximate the peak concentrations. A Student's t-test was used to compare mean values from field data and the model.

The first test of the model was to visually compare the model calculations with the observed data for each of the model segments. Figure 10-4 presents the phosphorus calculations. As seen here, the simulation of trends is reasonable, but variability in the data and model discrepancies do exist. This may be caused by short term variation not considered in the model or other factors. As an additional test, statistical analyses were performed.

The results of the statistical analysis are presented in Table 10-4 as percent of sampling cruises in which predicted and observed means were not significantly different at a 95 percent confidence level. Segments 1 and 3 had the lowest scores, but represent only 3.5 and 5.0 percent, respectively, of the total volume of the Bay. Also these are shoreline segments most influenced by changes in wind and tributary loading. Because segments 1 and 3 represent a small percentage of the total area, they were not emphasized in the calibration.

The model did a good job at matching total phosphorus despite large differences in total phosphorus concentrations among segments. The model was less effective in simulating the dissolved available phosphorus. Overall, the calibration resulted in approximately 86 percent of the model output being not significantly different than the field data for the thirteen principal variables.

Table 10-1. **Description of Model Coefficients [Bierman and Dolan (1981)].**

FACT	phytoplankton cell size in mg dry wt/cell
f(L)	phytoplankton light reduction factor (dimensionless)
f(T)	phytoplankton temperature reduction factor (dimensionless)
Ke	light extinction coefficient in meter^{-1}
KNCELL	intracellular half-saturation constant for nitrogen-dependent growth in moles N/cell
KPCELL	intracellular half-saturation constant for phosphorus-dependent growth in moles P/cell
KSCM	half-saturation constant for silicon-dependent growth of diatoms in moles Si/L
$KZSAT_k$	half-saturation concentration of phytoplankton for grazing by zooplankton **k** in mg/L
P, N	actual moles of phosphorus (nitrogen) per phytoplankton cell
PCA, NCA	intracellular available phosphorus (nitrogen) concentrations in moles/liter cell volume
PCAMIN, NCAMIN	minimum intracellular concentrations, corresponding to PSAMIN and NSAMIN, respectively, for available phosphorus (nitrogen) in moles/liter cell volume
PCM, NCM	concentrations of available nutrients (phosphorus, SCM nitrogen, silicon) in water column in moles/L
PDETH	maximum predatory death rate for zooplankton in liter/mg-day
PHOTO	photoperiod (dimensionless)
PKI, NKI	affinity coefficient for phosphorus (nitrogen) uptake mechanism in liters/mole
PO, NO	minimum cell quota of phosphorus (nitrogen) per phytoplankton cell in moles/cell
PSA, NSA	actual total phosphorus (nitrogen) in phytoplankton cells in moles/mg dry wt
PSAMIN, NSAMIN	minimum quota of phosphorus (nitrogen) in phytoplankton cells in moles/mg dry wt
$PSAT_k$	saturation concentration of zooplankton **k** above which predatory death rate remains constant, in mg/L
Q	water circulation rate in volume/day
RIPM, RINM	maximum phosphorus (nitrogen) uptake rate in day^{-1}
RADINC	incident solar radiation in langleys/day
RADSAT	saturation light intensity for phytoplankton growth in langleys/day
$RAGRZD_l$	rate at which phytoplankton **l** is ingested (grazed) by zooplankton in mg A/liter day
RAMAX	phytoplankton maximum growth rate at 20 C in day^{-1}
RLYS	phytoplankton decomposition rate in liter/mg day
RRESP	phytoplankton respiration rate in day^{-1}
RTOP, RTON, RTOS	rates of transformation from unavailable nutrient forms (phosphorus, nitrogen, silicon) to available forms in day^{-1}
RZ	zooplankton specific growth rate in day^{-1}
RZMAX	zooplankton maximum ingestion rate in day^{-1}
RZPEX, RZNEX, RZSEX	nutrient (phosphorus, nitrogen, silicon) excretion by zooplankton to unavailable nutrient pool in moles/mg zooplankton-day
SPGR	phytoplankton specific growth rate in day^{-1}
SSA	silicon composition of diatoms in moles/mg dry wt
T	temperature in C
CROP	total phytoplankton concentration in mg dry wt/L
TOP, TON, TOS	concentration of unavailable nutrient forms (phosphorus, nitrogen, silicon) in moles/L
TOPSNK, TONSNK, TOSSNK	sinking rates of unavailable nutrient forms (phosphorus, nitrogen, silicon) in meters/day
V	inner bay volume in liters
WPCM, WNCM, WSCM	external loading rates of available nutrients (phosphorus, nitrogen, silicon) in moles/day
WTOP, WTON, WTOS	external loading rates of unavailable nutrients (phosphorus, nitrogen, silicon) in moles/day
Z	zooplankton concentration in mg dry wt/L
ZASSIM	zooplankton assimilation efficiency (dimensionless)
$ZEFF_{kl}$	ingestion efficiency of zooplankton **k** for phytoplankton **l** (dimensionless)
ZDETH	specific zooplankton death rate in day^{-1}
ZKDUM	effective half-saturation concentration of total phytoplankton for grazing by zooplankton
ZSAFE	refuge concentration of zooplankton below which predatory grazing does not occur, in mg/L

NOTE: The addition of the suffix "BD" to a variable refers to the boundary value of the variable.

Table 10-2. Summary of Selected Model Coefficients [Bierman and Dolan (1981)].

a. Summary of Phytoplankton Coefficients

Coef.	Units	Diatoms	Greens	Others	Blue-Greens (non-N_2)	Blue-Greens (N_2-Fixing)
R1PM	day^{-1}	0.500	0.500	0.500	0.500	0.500
PK1	liters/mole	0.518×10^{6}	0.167×10^{7}	0.158×10^{6}	0.200×10^{7}	0.518×10^{6}
PO	mole P/cell	0.724×10^{-13}	0.312×10^{14}	0.148×10^{-13}	0.566×10^{14}	0.488×10^{14}
CONCP		0.250×10^{6}	0.250s10^{6}	0.250×10^{6}	0.356×10^{6}	0.356×10^{6}
KPCELL	mole P/cell	0.724×10^{-13}	0.312×10^{-14}	0.148×10^{-13}	0.566×10^{-14}	0.488×10^{-14}
RINM	day^{-1}	0.125	0.125	0.125	0.125	0.125
NKI	liters/mole	0.100×10^{7}	0.100×10^{7}	0.100×10^{7}	0.100×10^{7}	0.100×10^{7}
NO	mole N/Cell	0801×10^{-11}	0.345×10^{-12}	0.163×10^{-11}	0.438×10^{-12}	0.377×10^{-12}
CONCN		0.208×10^{7}	0.208×10^{7}	0.208×10^{7}	0.208×10^{7}	0.208×10^{7}
KNCELL	mole N/cell	0.801×10^{-11}	0.345×10^{-12}	0.163×10^{-11}	0.438×10^{-12}	0.377×10^{-12}
SSA	mole Si/mg	0.334×10^{-5}				
KSCM	mole Si/liter	0.357×10^{-5}				
RAMAX	day^{-1}	1.6	1.4	1.2	1.0	0.70
ASINK	meter/day	0.05	0.05	0.05	0.05	0.05
RLYS	liters/mg/day	0.004	0.004	0.004	0.012	0.012
FACT	mg/cell	0.450×10^{-5}	0.194×10^{-6}	0.918×10^{-6}	$0.246.10^{-6}$	0.212×10^{-6}
RADSAT	langleys/day	100	100	100	50	50
RRESP	day^{-1}	0.05	0.05	0.05	0.05	0.05

b. Summary of Zooplankton Coefficients

Coef.	Unit	Faster Ingester	Slow Ingester
RZMAX	day^{-1}	0.70	0.10
ZASSIM		0.60	0.60
$KZSAT_k$	mg/liter	1.0	1.0
AZMIN	mg/liter	0.20	0.20
BDETH	day^{-1}	0.05	0.01
PDETH	day^{-1}	0.50	0.10
ZSAFE	mg/liter	0.01	0.01
$PSAT_k$	mg/liter	1.0	1.0

c. Summary of Coefficients for Unavailable Nutrients

Coefficient	Units	Value
RTOP, RTON,	day^{-1}	0.005
RTOS, TOPSNK, TONSNK	meters/day	0.05

10.3.4. Projections

In a report to the International Joint Commission (Bierman and Dolan, 1980) the model was applied to seven scenarios of phosphorus loadings. The scenarios consisted of various combinations of advanced wastewater treatment and non-point source reduction. The results were presented as annual average total phosphorus concentration, total phytoplankton biomass, total blue-green phytoplankton biomass, and taste and odor in the municipal water supply. Although the Bay was partitioned into five segments, only two contrasting segments (segments 2 and 4) were analyzed. Segment 2 contained 73 percent of the total water volume of the inner Bay and was the most degraded portion of the Bay. Segment 4 had the highest water quality in the Bay. These segments represented the two extremes in the Bay.

In the model simulations, peak total biomass concentrations did not change significantly with reductions in phosphorus loads; however, the blue-green phytoplankton responded in direct proportion to phosphorus reduction in segment 2 and in a lower proportion in segment 4. This was the first objective of nutrient control in the Bay.* This simulation of algal species change is a unique aspect of this multi-class phytoplankton model. The model has the ability to distinguish nutrient limitation among different types of phytoplankton and hence allows changes in composition.

In general, the model showed phytoplankton growth to be nitrogen-limited, but for a two month period (May and June) diatoms were silica-limited. This agreed with actual observations of nutrient depletion. In mid-August, the nitrogen-fixing blue-greens capitalized on the depletion of nitrogen and proliferated. Their growth was then restricted by phosphorus limitation.

* Later application of the model to 1980 data in a post-audit shows the blue-greens actually responded in a much greater proportion to phosphorus reduction.

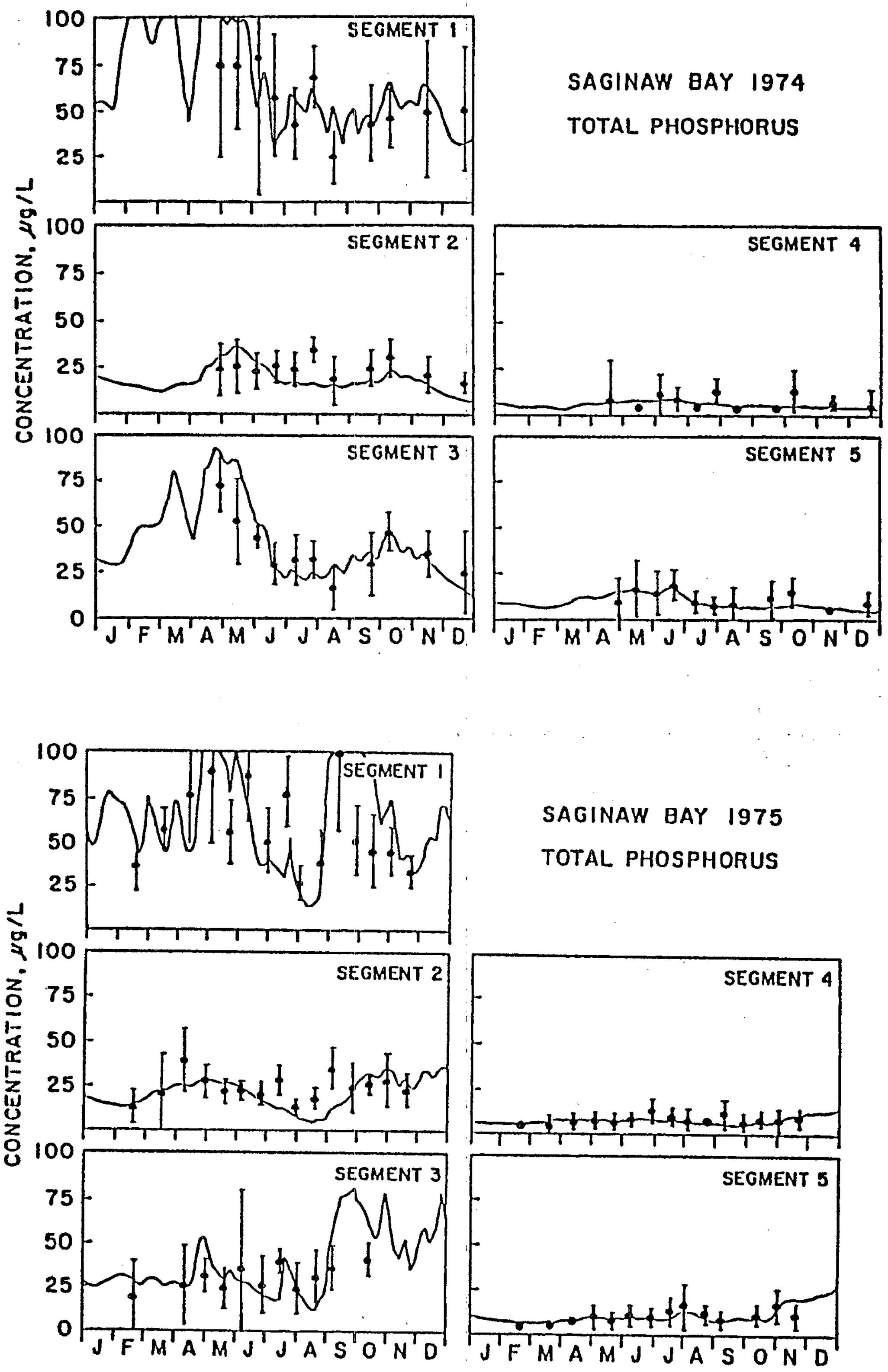

Figure 10-4. **Model output and field data comparison for total phosphorus (solid line is model output; data are sampling cruise means and three standard deviations) [Bierman and Dolan (1986a). Reprinted from ASCE Journal of Environmental Engineering, Vol. 112, No. 2. p. 409. With permission].**

Table 10-3. Summary of Selected Model Inputs [Bierman and Dolan (1986b). Reprinted from ASCE Journal of Environmental Engineering, Vol. 112, No. 2. p. 422. With permission].

Parameter	Sample Year		
	1974	1975	1980
Saginaw River Loadings (Metric Tons):			
Total Phosphorus	1266	1470	493
Total Nitrogen	14,100	15,290	11,030
Total Silicon	23,000	31,000	12,250
Environmental Forcing Factors:			
Number of Days Where Wind Speed Exceeded Threshold for Resuspension (Annual)	29	40	35
Annual Average Water Temperature (°C)			
Segment 2	12.0	13.9	14.9
Segment 4	9.8	11.1	12.8

10.4. Post-Audit

In 1980, a survey was conducted and used in a post-audit of the model. A post-audit provides a test of the model for use in projections by comparing forecasts to actual observations. Environmental conditions changed substantially in five years. From 1975 to 1980, total annual load of total phosphorus decreased 66 percent and available phosphorus decreased 78 percent. It was estimated that 44 percent of the drop in phosphorus load was because of decreases in tributary flow. The other 56 percent was attributed to point source controls and a detergent phosphorus ban for the State of Michigan initiated in 1977. Total phytoplankton biomass also decreased substantially, with the nitrogen-fixing blue-greens being nearly eliminated.

The predictive capability of the model was tested using the 1980 data. The model was rerun using the 1974 and 1975 model coefficients but loading and environmental conditions for 1980. The results are presented as a comparison of predicted and observed percent reductions between the 1974-75 calibration years and the 1980 resurvey year (Figure 10-5). In general, the model overestimated the percent reduction in total phosphorus, and underestimated reductions in diatoms and blue-green algae.

Table 10-4. Statistical Comparison between Model Results and Field Data [Bierman and Dolan (1986b)].

Year	Cell*				
	1	2	3	4	5
1974	72	85	65	88	87
1975	64	80	72	86	87
1980	57	64	52	85	86

* Percent of sampling cruises for which computed mean values not significantly different from observed mean values at 95% confidence level; average of 13 variables.

Underestimation of phosphorus concentrations was a characteristic of model results during the calibration years and in the post-audit survey. This discrepancy was attributed to the underestimation of wind-driven resuspension of sediments. Nevertheless, the model's prediction of elimination of threshold odor violations at the water treatment plant agreed with the data. This was the primary management need for the model. Blue-green phytoplankton biomass in segment 4 was correlated with threshold odor in the drinking water intake. The model predictions for threshold odor violations in the drinking water intake agreed with observations because both were below the blue-green biomass threshold.

Overall, the model predictions did not match observed concentrations closely, but were consistent with observed trends. The model correctly predicted that if phosphorus loadings were reduced to 400-500 metric ton/year, blue-green algae would decrease more than other species and threshold odor would be eliminated. The response of the blue-greens exceeded the prediction of the model in absolute values.

10.5. References

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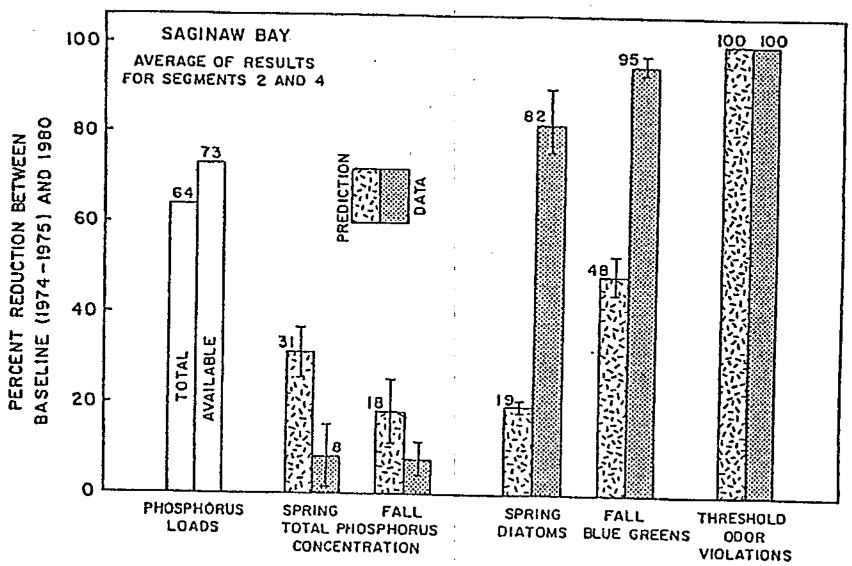

Figure 10-5. Changes in water quality constituents between 1974 and 1980 in segments 2 and 4 [Bierman and Dolan (1986b). Reprinted from ASCE Journal of Environmental Engineering, Vol. 112, No. 2. p. 409. With permission].

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11. Potomac Estuary Water Quality Modeling

11.1. Background

The studies discussed here include application of three different waste load allocation-related models for the Potomac Estuary near Washington, D.C. The three models, although covering basically the same location, have markedly different structures to address three different water quality issues. The water quality concerns consisted of:

- Dissolved Oxygen Depression
- Nutrient Enrichment and Algal Proliferation
- Total Residual Chlorine

These three water quality concerns each had unique spatial and temporal considerations, such that all concerns could not be properly addressed by a single model. In this regard, three separate (but inter-related) models were developed to specifically address each issue. The Dynamic Estuary Model (DEM), a one-dimensional, spatially detailed real-time dissolved oxygen model was applied to determine effluent limitations for oxygen-demanding materials. The Potomac Eutrophication Model (PEM), a tidally-averaged eutrophication model, was applied to determine the impact of nutrient control strategies on regional algal concentrations. Neleus, a real-time, two-dimensional finite element model, was applied to determine very localized total residual chlorine impacts and the potential for forming a barrier to fish passage.

11.2. Problem Setting

The Potomac Estuary drains an 11,560 square-mile area, comprising portions of Maryland, Virginia, West Virginia, and Pennsylvania. It is used for a wide variety of activities, ranging from industrial water supply (primarily cooling water supplies), to navigation, boating and commercial and sport fishing.

The Potomac Estuary extends 114 miles from the fall line at Chain Bridge in Washington, D.C. to its junction with the Chesapeake Bay (see Figure 11-1). The es-

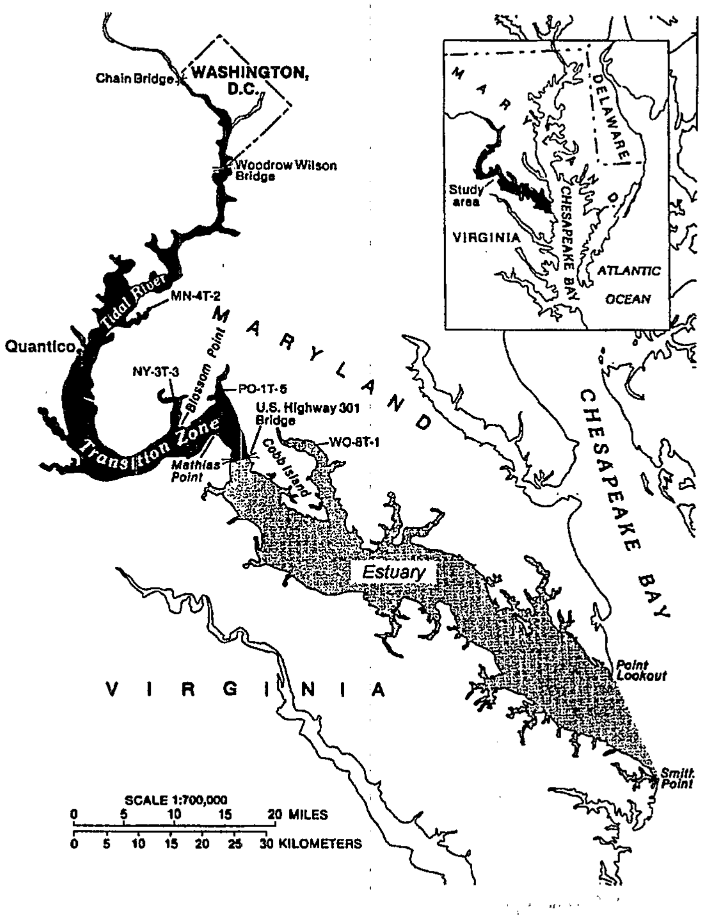

Figure 11-1. Location map of Potomac Estuary [USGS (1985)].

tuary can be divided into three zones: the freshwater or tidal river zone, the transition zone, and the saline zone. The upper reach, although tidal, contains only freshwater, and extends from Chain Bridge to just above Quantico. The middle zone is characterized by a transition from fresh to brackish water and extends from Quantico to the Highway 301 bridge. The lower reach is highly saline, vertically stratified, and often anoxic near the bottom. The modeling and waste load allocation discussed herein focuses on the freshwater zone.

The major source of pollutants in the upper Potomac Estuary is the District of Columbia and its suburbs. Population in the Washington, D.C. area increased from 2.1 million in 1960 to 3.2 million in 1980. At least 14 wastewater treatment plants with a combined flow well over 500 MGD discharged into the Potomac Estuary in 1980. This discharge is a significant increase over the 325 MGD wastewater flow in 1966. While effluent flow has increased, the load of phosphorus and BOD_5 from these point sources has decreased approximately seventy-five and fifty per cent respectively during this period because of substantial improvements in wastewater treatment.

The most significant point source discharge to the estuary is the Blue Plains Wastewater Treatment Plant in Washington, D.C., which has an average annual flow of 227 MGD. Other sources of nutrients and oxygen demanding material to the Potomac Estuary include nonpoint source discharges from upper basin drainage and downstream tributaries, combined sewer overflows, and atmospheric pollutants.

The upper portion of the Potomac Estuary has been plagued with occurrences of low levels of dissolved oxygen, floating algal mats, and high concentrations of chlorophyll *a*, indicating a relatively advanced state of eutrophication. In recent years, these problems have dramatically declined because of increased wastewater treatment.

11.3. Dynamic Estuary Model (DEM) of Dissolved Oxygen

The Potomac Estuary was regularly depleted of dissolved oxygen during the 1960s and early 1970s in response to point sources of pollution and combined sewer overflows in the Washington, D.C. area. U.S. EPA Region III, in their "Potomac Strategy", highlighted the need to develop and validate water quality models for the Potomac that could be used for waste load allocation purposes (Clark, 1982). The Potomac Strategy State/EPA Technical Committee subsequently recommended DEM as the appropriate model to use to assess dissolved oxygen impacts in the Upper Potomac. Their decision was, in large part, based on the capability of the model to provide good spatial resolution and diurnal calculations.

DEM represents the Potomac using a series of interconnected channels and junctions. These channels and junctions can be arranged to simulate simple two-dimensional features of the estuary, but are primarily one-dimensional (i.e. no lateral variation) with branching. DEM as configured for the Potomac extends from Chain Bridge (River Mile 0.0) as an upstream boundary to Piney Point (River Mile 96.2) as a downstream boundary. This configuration consists of 133 junctions and 139 channels, but the focus of the water quality modeling was in the upper 20 miles. DEM simulates in "real time", meaning that the model predicts conditions as they vary through diurnal and tidal variations.

DEM consists of two separate but closely related models. The first, a hydrodynamic model, simulates both the tidal and net advective movement of water. This model provides predictions of water depth, velocity, and direction of flow based upon input information on geometry, roughness, tributary inflows and tidal variations in depth at Piney Point. The results of the hydrodynamic model are input to the second model, which simulates water quality.

The water quality model predicts the transport and transformation of pollutants in the Potomac Estuary. The model, as applied for Potomac dissolved oxygen, simulates three variables: dissolved oxygen, carbonaceous biochemical oxygen demand (CBOD), and ammonia.

Dissolved oxygen concentrations are increased by atmospheric reaeration and algal photosynthesis, and are decreased by oxidation of CBOD, nitrification of ammonia, sediment oxygen demand, and algal respiration. The model does not predict algal photosynthesis or respiration. Instead, these values must be input by the modeler based upon observed data or calculations performed external to the model. CBOD concentrations are increased by point and nonpoint loadings, and are decreased by settling and deoxygenation of CBOD. Ammonia concentrations are increased by point and nonpoint loadings, and are decreased by a first-order loss term defined in DEM as nitrification.

Water quality data for model calibration and verification consisted of both wet and dry weather surveys conducted in 1965, 1966, 1967, 1968, 1970, 1977, 1978, 1979, and 1980. The Blue Plains Wastewater Treatment Plant, the primary point source of pollutants to the river, implemented secondary treatment in 1977.

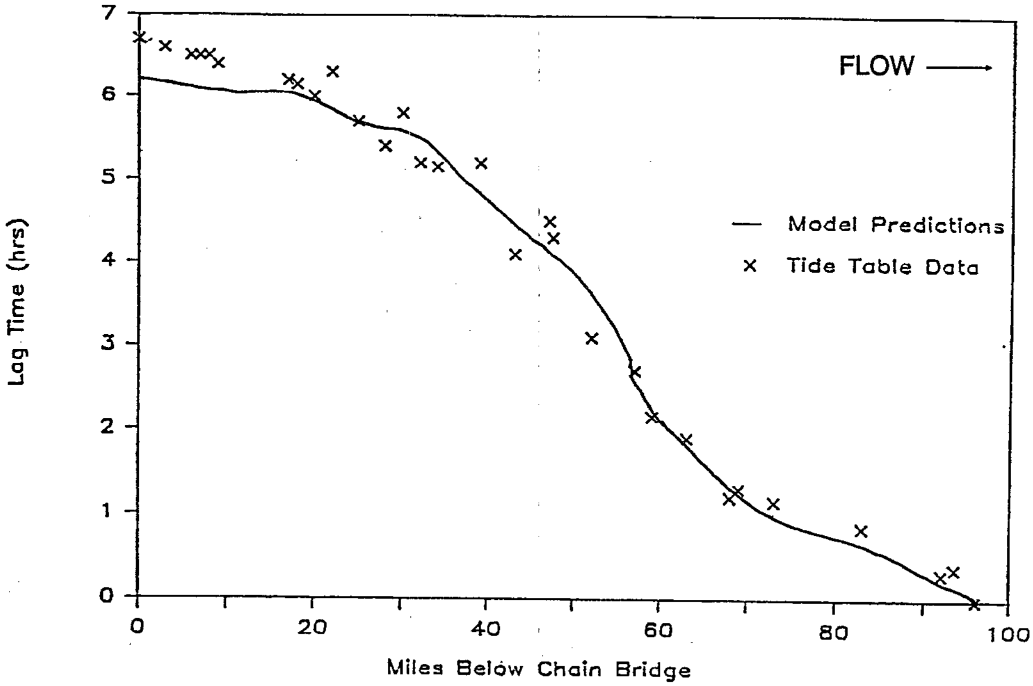

Figure 11-2. Potomac Estuary hydraulic calibration high water phasing — Mean Tide [Adapted from Clark (1982)].

11.3.1. Model Calibration/Verification

Calibration of DEM to the Potomac required separate calibration of both the hydrodynamic and water quality submodels. Hydrodynamic calibration focused on the channel roughness coefficient to best describe the magnitude and phasing of predicted tides. The model was calibrated using mean upstream freshwater flow (11,000 cfs) and elevation data published in the National Oceanographic and Atmospheric Administration (NOAA) Tide Tables. Sample model calibration results are shown in Figure 11-2. The hydrodynamic submodel was then verified to observed data from the periods January 11-13, 1971 and July 22-28, 1981. The calibrated roughness coefficients accurately reproduced tidal range and phasing for all data sets.

The water quality submodel calibration was divided into two separate tasks: 1) calibration of dispersion (using conservative tracers) and 2) calibration of reaction rate coefficients (using water quality concentrations). The dispersive transport coefficient was calibrated to chloride data collected during the period August 1 to September 8, 1977, and verified to chloride data from the period September 15 to November 12, 1969. The model predicted the majority of data quite well, but was unable to simulate the steepest portion of the chloride gradient due to numerical dispersion (Figure 11-3). The dispersion rates determined through calibration and verification of the chloride data were also tested against a 1978 dye survey. The model was able to simulate observed far-field data quite well, with discrepancies in near-field embayments.

Water quality data for model calibration of reaction kinetics consisted of surveys conducted in 1965, 1966, 1967, 1968, 1970, 1977, 1978, and 1979. The objective of the calibration procedure was to simulate as many data sets as possible and to provide a test of the model's ability to duplicate a wide range of conditions. Model calibration (coefficient adjustment) was conducted on data sets through 1977, with the later data sets used for verification (without coefficient adjustment). The data sets from 1965 to 1970 were collected during periods of relatively constant environmental conditions and used for steady-state model comparisons. The 1977 data set was collected over a two month period characterized by a massive algal bloom (100-300 ug/l chlorophyll *a*) and die-off, and used a real-time model to characterize the significant transient processes. Example model calibration to data is shown in Figures 11-4 to 11-6 for the parameters ammonia, nitrate + nitrite, and dissolved oxygen. Comparisons of BOD were not provided because algae complicated its measurement and comparisons. The model generally reproduced trends in observed data quite well and was also very successful in matching 1978 and 1979 data during model validation.

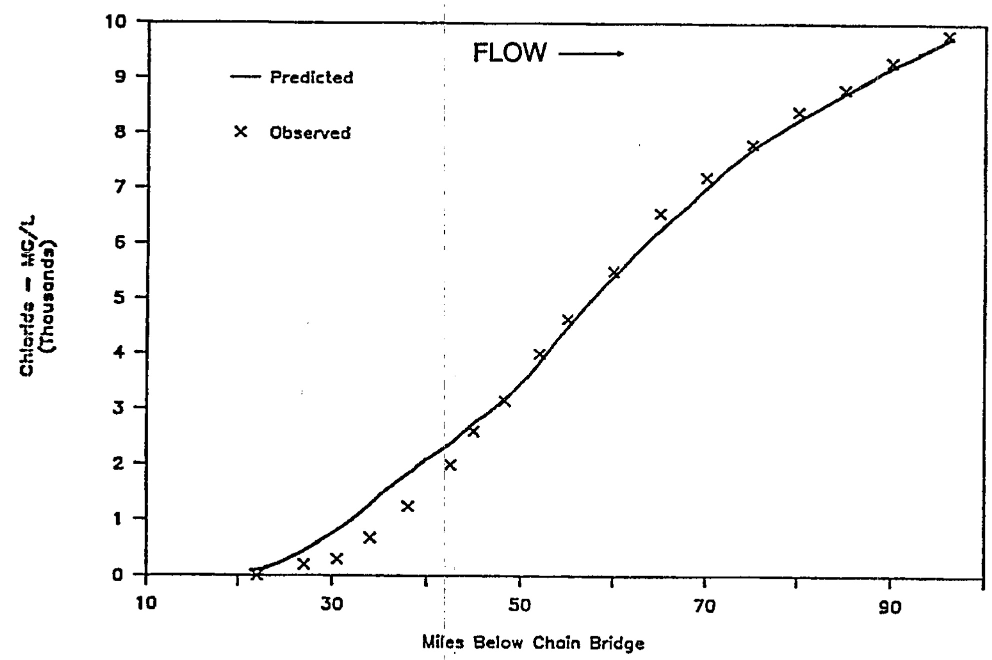

Figure 11-3. Potomac Estuary chloride verification, time period: September–October, 1969 [Adapted from Clark (1982)].

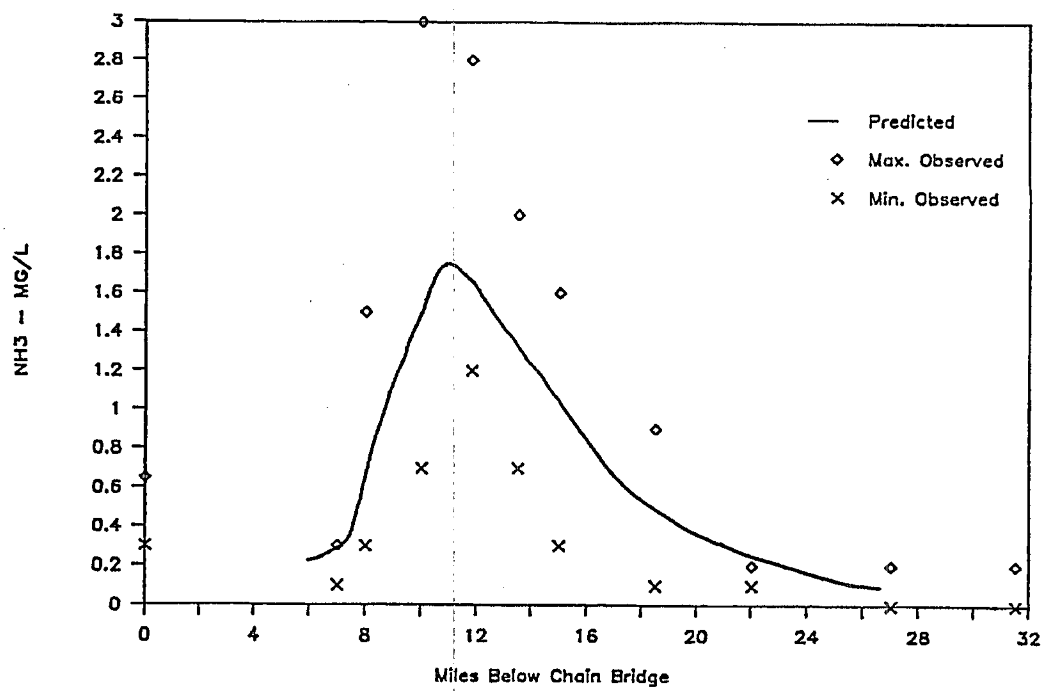

Figure 11-4. DEM calibration results for ammonia, time period: August 31–September 16, 1965 [Adapted from Clark (1982)].

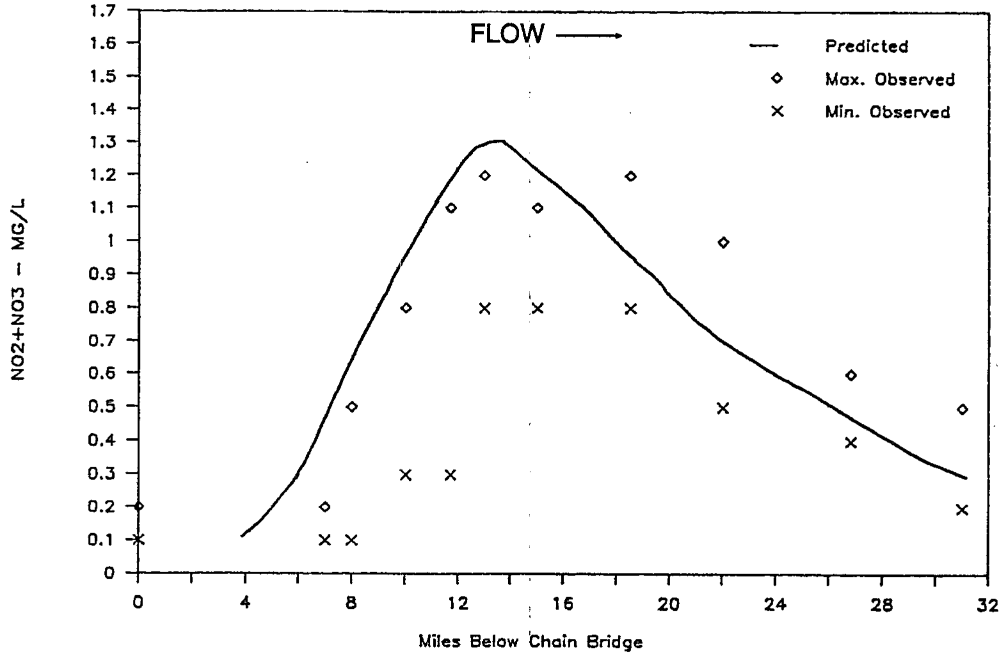

Figure 11-5. DEM calibration results for nitrate+nitrite, time period: August 31–September 16, 1965 [Adapted from Clark (1982)].

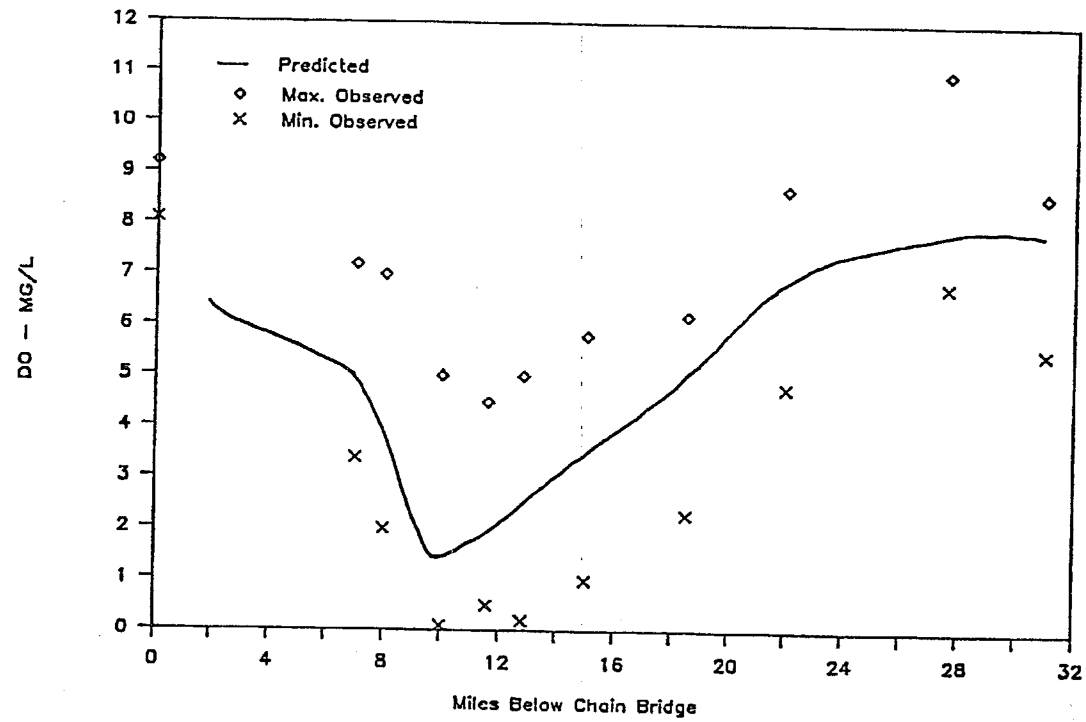

Figure 11-6. DEM calibration results for dissolved oxygen, time period: August 31–September 16, 1965 [Adapted from Clark (1982)].

11.3.2. Model Application

Application of DEM was conducted over the course of several years and modeling efforts. Initial waste load allocation projections were made by U.S. EPA (Clark, 1982). A revised and updated examination was performed in 1984, but recommendations from this effort were deferred when data from the mid-1980's appeared inconsistent with model predictions (MWCOG, 1987). The model was then revalidated in 1987 to more recent water quality data, and new waste load allocation projections performed.

DEM was applied by Greeley and Hansen (1984) as part of the Washington D.C. Blue Plains Feasibility Study, to determine regional capacity treatment needs and establish allowable effluent loads for dischargers to the Upper Estuary. Numerous alternatives were examined for water quality compliance and other factors. Seven final regional wastewater treatment scenarios were evaluated for their ability to lead to compliance with water quality standards for dissolved oxygen. Model projections were made at critical environmental conditions consisting of drought (7Q10) freshwater flow and a water temperature of 28°C, the upper 90th percentile temperature at summer low flow. Model coefficients were based on the average of post-1977 simulations. Algal productivity and respiration inputs were derived from drought flow simulations using the Potomac Eutrophication Model (see later discussion). Sediment oxygen demand (SOD) was proportionately reduced with loadings toward background values. Boundary concentrations were representative of the period 1977-1979.

DEM model results for both daily averaged and daily minimum dissolved oxygen indicated that all final alternatives evaluated would lead to compliance with dissolved oxygen standards for the critical conditions scenario. Water quality differences between scenarios were viewed as small in comparison to the substantial differences in cost. The recommended treatment scenario was subsequently based upon cost, engineering and other considerations.

11.3.3. DEM Post Audit

State and Federal regulators originally rejected the DEM-based waste load allocation recommendations, due primarily to a review of 1982-1985 dissolved oxygen data from the Upper Potomac. These data indicated that dissolved oxygen standards violations were still occurring, even though treatment plants were performing at recommended levels. Given that DEM predicted that additional nitrification treatment at two area POTWs would improve minimum dissolved oxygen concentrations by 0.8 mg/l, they recommended nitrification treatment at these plants.

Local governments expressed considerable reservation regarding the need for improved treatment, and conducted a study to revisit the DEM modeling analysis and examine regulatory agency concerns (MWCOG, 1987). Extensive water quality surveys were conducted in the Upper Potomac in 1986 to validate (or refute) the predictive capability of DEM. In addition, special studies were conducted investigating current pollutant decay rates, sediment oxygen demand, and occurrence and cause of water quality standard violations. Limno-Tech (1987) applied DEM to simulate 1985 and 1986 conditions. This analysis determined that DEM calculations of dissolved oxygen were very sensitive (±3 mg/l) to algal-productivity related parameters which were not directly measured. Given judicious selection of inputs, DEM could simulate recent dissolved oxygen data. Since neither observed (nor eutrophication model predicted) algal productivity information was available, DEM predictions could not be explicitly confirmed or refuted. An important outcome of this analysis was that transient changes in algal productivity could be responsible for dissolved oxygen standards violations, irrespective of point source impacts. Furthermore, detailed examination of DEM indicated that it over-calculated the benefits from additional nitrification treatment because it simplistically assumed all ammonia loss was due to nitrification. The ammonia mass balance is a net combination of nitrification, algal uptake of ammonia, sediment ammonia release, and hydrolysis of organic nitrogen. Re-evaluation indicated a reduced nitrification rate and a benefit due to additional nitrification treatment of 0.2 to 0.5 mg/l.

As a result of these findings, the dominance of net algal productivity and the small benefits from additional nitrification treatment, further nitrification treatment requirements were deferred.

11.4. Potomac Eutrophication Model (PEM)

The Potomac Estuary began exhibiting signs of eutrophication (algal blooms, floating mats of vegetation) in the late 1940s and continued through the 1960s. In an effort to control these problems, point source discharges of total phosphorus to the estuary were reduced by seventy-five percent over the period 1968 to 1979. However, algal bloom conditions persisted into the late 1970's, causing concern as to whether the decrease in point source phosphorus was controlling eutrophication. The Potomac Eutrophication Model (PEM) was developed to determine the impact of historical pollution controls on Potomac Estuary eutrophication, and to guide regulators in setting future effluent limitations.

The PEM model was developed because the existing DEM model focused more on spatial resolution than on the kinetic complexities of eutrophication which were necessary to forecast the benefits of nutrient controls. In addition, the tidally averaged and large segment approach of PEM is more consistent with the regional and seasonal focus of eutrophication. PEM is a version of the EPA supported Water Quality Analysis Simulation Program (WASP), but developed specifically for the Potomac (Hydroqual, 1982). Compartment or box modeling techniques are used to represent the estuary as a series of water column and sediment segments. There is no hydrodynamic submodel included in PEM. Average flows, velocities, and dispersion coefficients are not computed by the model; they are specified as model inputs. The hydrodynamic inputs are tidally averaged and reflect seasonal changes, not daily or hourly changes. The kinetic equations employed in PEM link phytoplankton growth and death to non-linear nutrient interactions and recycle mechanisms, directly couple phytoplankton to dissolved oxygen concentrations, and internally compute sediment nutrient release and oxygen demand. The following state variables are included in PEM:

- Chlorides
- Phytoplankton carbon
- Total organic nitrogen
- Ammonia nitrogen
- Nitrite-nitrate nitrogen
- Dissolved and particulate organic phosphorus
- Dissolved and particulate inorganic phosphorus
- Carbonaceous biochemical oxygen demand
- Dissolved oxygen

PEM computes water column concentrations on a daily basis. The focus in calibrating the model was on matching monthly and annual trends over a regional scale of 75-100 miles. Such spatial and temporal scales represent the global response of the estuary to seasonally transient nonpoint source inputs from the upper Potomac Basin and tributaries, and point sources from wastewater treatment plants.

The PEM network consists of 23 main channel segments and 15 tidal embayment segments, each with a sediment layer segment below. These segments range in length from one to two miles in the upper tidal freshwater portion of the estuary, to 10-15 miles in the lower, saline portion of the estuary. The focus of the modeling was on the freshwater segments.

11.4.1. Model Calibration/Verification

Historical data from several sources were used for both the calibration and verification of PEM. Data sets were selected that provided spatial coverage of at least the upper 50 miles of the estuary on a biweekly or monthly basis for the crucial summer period, and that included simultaneous measurements of chlorophyll *a*, nutrients, and dissolved oxygen. Data from different sources were often combined to produce a more robust characterization of the estuary. The data sets generally had biweekly sampling during the warm weather season at stations 1 to 2 miles apart in the freshwater portions of the upper estuary. Data collected during 1966, and 1968 through 1970 were used in the calibration, and are representative of water quality conditions prior to the implementation of phosphorus removal at the major sewage treatment plants along the estuary.

USGS data from the years 1977 through 1979 were used to verify PEM. These years were selected because they offered the chance to study the changes in the estuary after institution of phosphorus removal at Blue Plains. Thus, the verification period provided an opportunity to further test the model's ability to simulate the eutrophication process in the Potomac Estuary.

The verification data set involved short, intensive week-long surveys in 1977 and 1978. The entire length of the estuary was usually sampled twice during the 1977 and 1978 surveys, with vertical samples collected at a number of stations. In 1979, the spatial and temporal coverage was reduced, and sampling was limited to twice a week at five major stations.

11.4.2. Environmental Inputs

The PEM application for 1966 to 1979 required extensive inputs for environmental conditions including flows, loads, and boundary conditions which are summarized below.

PEM does not include a hydrodynamic submodel, so flows must be input for each segment of the model. To simplify model input during the calibration period, only the two major and dominant sources of freshwater flow were included, the Potomac River at Little Falls (the upstream boundary) and the Blue Plains Wastewater Treatment plant effluent. Downstream tributary flows and other treatment plant discharges were deemed minimal. Both upstream freshwater flows and Blue Plains effluent flows were input to the model using piece-wise linear approximations of seasonal flow patterns, not actual day-to-day fluctuation. For model verification, the model also included flows for the Anacostia River and Occoquan Reservoir. These flows were insignificant during the extreme drought of the calibration period, but were of sufficient magnitude during verification that they had to be considered.

Pollutant loads to the Potomac were divided into three categories: 1) Point Sources, 2) Combined Sewer Overflows, and 3) Nonpoint Sources. Point source inputs of pollutants were defined by monitoring data and daily operating reports from the area's municipal wastewater treatment plants. The Blue Plains treatment facility accounted for the large majority of these inputs.

In addition to permitted outfalls, an unregulated "gap" in a major sewer line contributed approximately 6 MGD of raw sewage until closed in July 1972. Estimates of monthly averaged combined sewer overflow pollutant loadings for Washington D.C. were generated with a SWMM model simulation of the D.C. sewer network. Combined sewer overflows for Alexandria were estimated based on calculated stormwater runoff and the average CSO concentrations measured in the D.C. sewer system.

Nonpoint source loads to the estuary were estimated for all tributaries to the main stem of the Upper Potomac Estuary. The nonpoint source flow for each tributary was based on data from USGS gaging stations. Estimates of flow for ungaged tributaries were based on the gaged discharge in neighboring tributaries. Seasonal flow trends were defined for each year by smoothing out many of the small peak flows using linear approximations. Water quality concentrations associated with nonpoint runoff were based on predictions of the Nonpoint Source (NPS) model. Simulated daily flows and pollutant loadings from 1977 to 1979 were analyzed, and a mean concentration for each of three flow ranges were determined and used in the model inputs. Slight reductions in concentrations were used for the 1960's simulations to reflect the less developed land use.

11.4.3. Boundary Conditions

Model inputs for upstream boundary conditions were based on data but required considerable extrapolation and interpolation to simulate the several years of conditions. Available data were statistically analyzed and correlated to flow. Where applicable, relationships were used between pollutant concentration (e.g. nitrate) and flow; otherwise, average concentrations were matched to observed USGS flow. All inputs were smoothed to characterize seasonal trends, not day to day transients.

11.4.4. Calibration

The model calibration included reaction rates for phytoplankton growth, nitrogen and phosphorus cycling, and the distribution of CBOD and dissolved oxygen. Calibration was accomplished by varying rate coefficients until a satisfactory fit was obtained between the predicted and observed water quality data. Model coefficients were identical for all calibration surveys. External inputs such as flow, temperature, solar radiation, and light extinction coefficients were as measured during the surveys.

Figures 11-7 to 11-10 show predicted and observed water quality data. These figures present calibration results for chlorides, chlorophyll *a*, DO, BOD_5, total organic phosphorus, total inorganic phosphorus, ammonia nitrogen, and nitrite-nitrate nitrogen during May and September of 1966, the year with the lowest recorded flow. The model predicted the overall variation in the data well. Of particular note is the chloride calibration, which validated water transport. Other calibration runs were similar.

11.4.5. Verification

Initial verification used 1977-1979 environmental conditions and the model coefficients derived during calibration. Some of the calibrated coefficients had to be modified for the verification period to reflect improved treatment and the altered settling characteristics of inorganic phosphorus. These changes included the relocation of the Blue Plains outfall and the use of ferric chloride to precipitate phosphorus. To account for the altered settling characteristics, a spatial settling function was developed that was unique to the verification. The instream nitrification rate and the oxidation rate for carbonaceous BOD were also changed to reflect improved treatment levels.

Predicted and observed water quality are compared in Figures 11-11 and 11-12, which illustrate the July 1977 PEM verification for chlorides, chlorophyll *a*, dissolved inorganic phosphorus, total phosphorus, ammonia nitrogen, nitrite-nitrate nitrogen, BOD_5 and DO. Similar results were attained for other surveys.

11.4.6. Statistical Assessment of Validation

In addition to the graphical comparisons, statistical measurements of goodness-of-fit tested the adequacy of PEM for future predictions. The three statistical procedures used in the PEM study are:

- Regression analyses
- Relative error
- Comparison of means.

In regression analyses, the calculated values from the model are compared to the observed values, and a number of standard statistics computed, including the correlation coefficient and the standard error of the estimate. Table 11-1 shows that 73 to 88 percent of the variability in the observed chlorophyll *a* data and 60 to 93 percent of the variability in the observed dissolved oxygen are explained by the model.

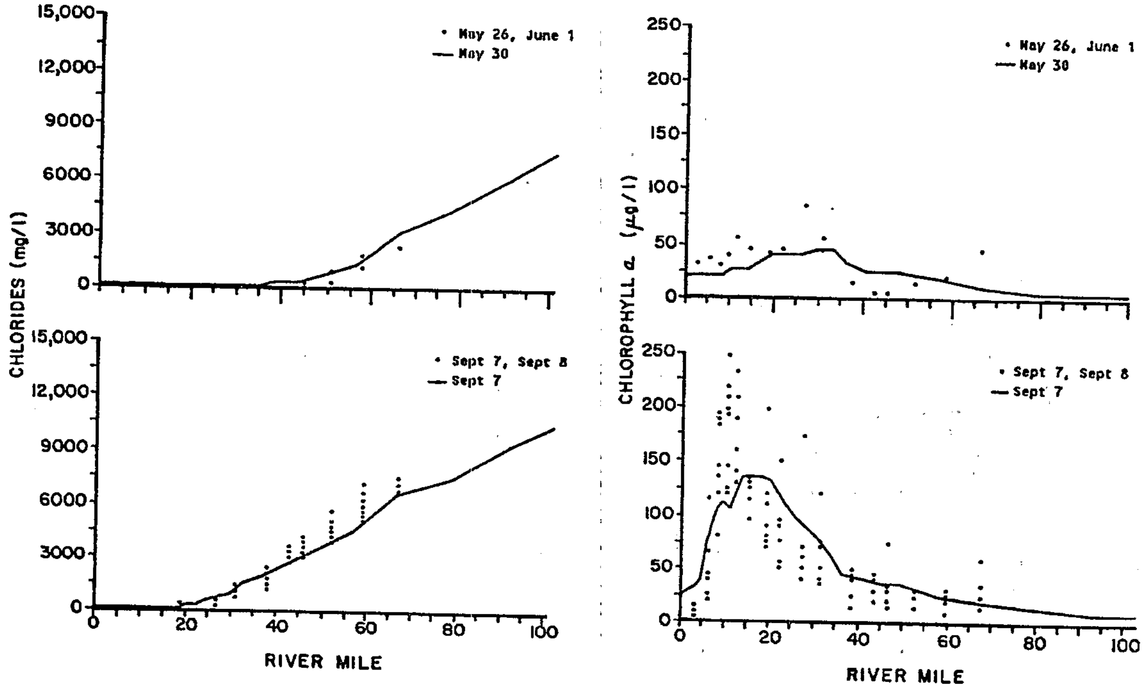

Figure 11-7. PEM calibration for chlorides and chlorophyll a, May and September, 1966 [Hydroqual (1982)].

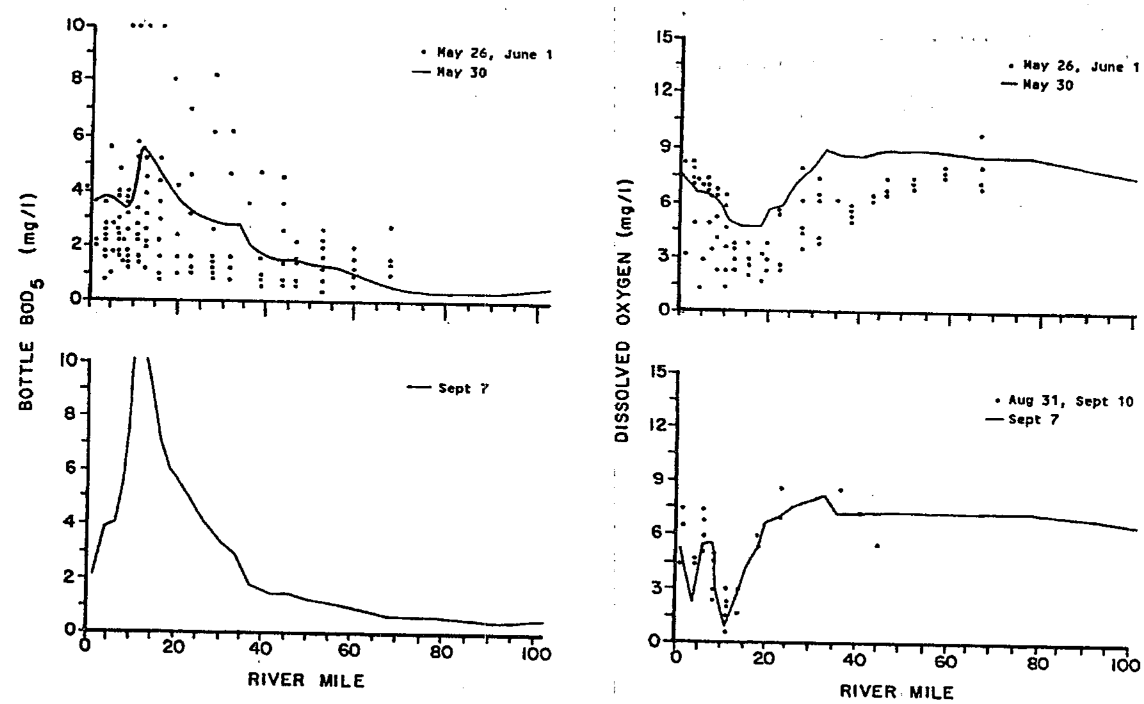

Figure 11-8. PEM calibration for BOD5 and dissolved oxygen, May and September, 1966 [Hydroqual (1982)].

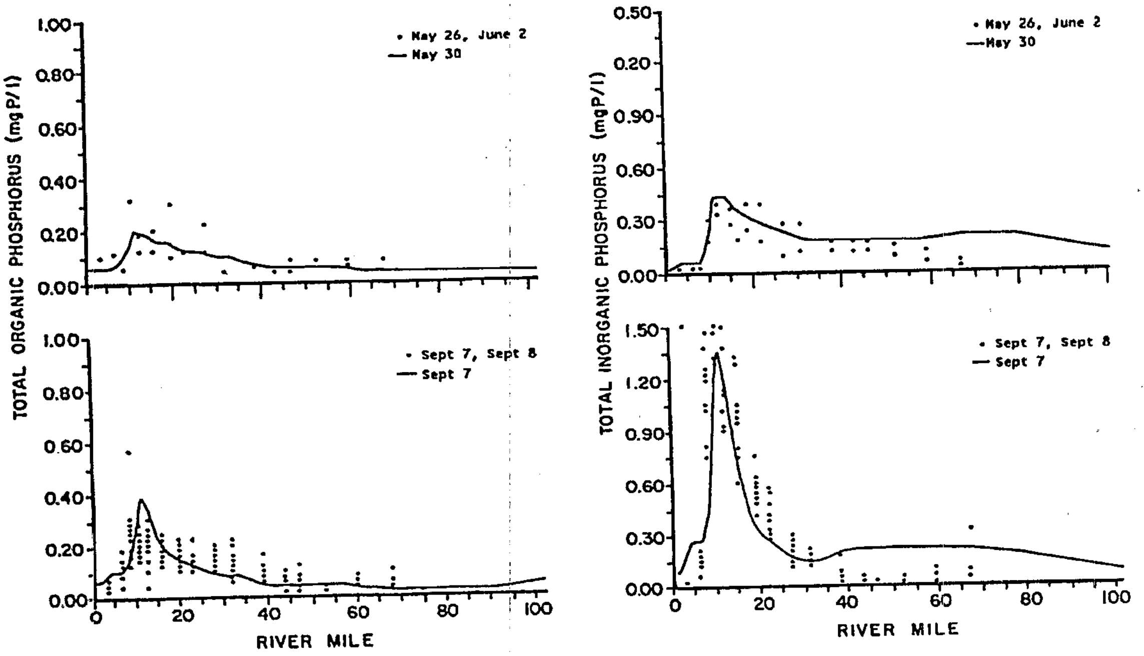

Figure 11-9. PEM calibration for total organic and total inorganic phosphorus (mg P/L), May and September, 1966 [Hydroqual (1982)].

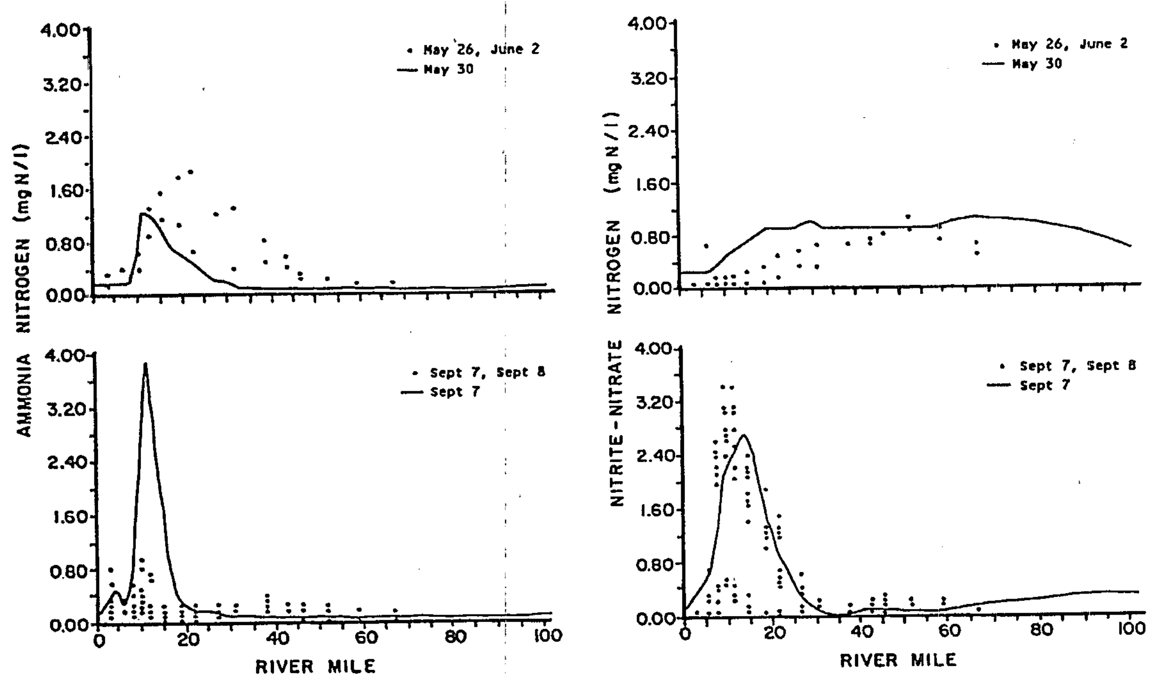

Figure 11-10. PEM calibration for ammonia and nitrite+nitrate (mg N/L), May and September, 1966 [Hydroqual (1982)].

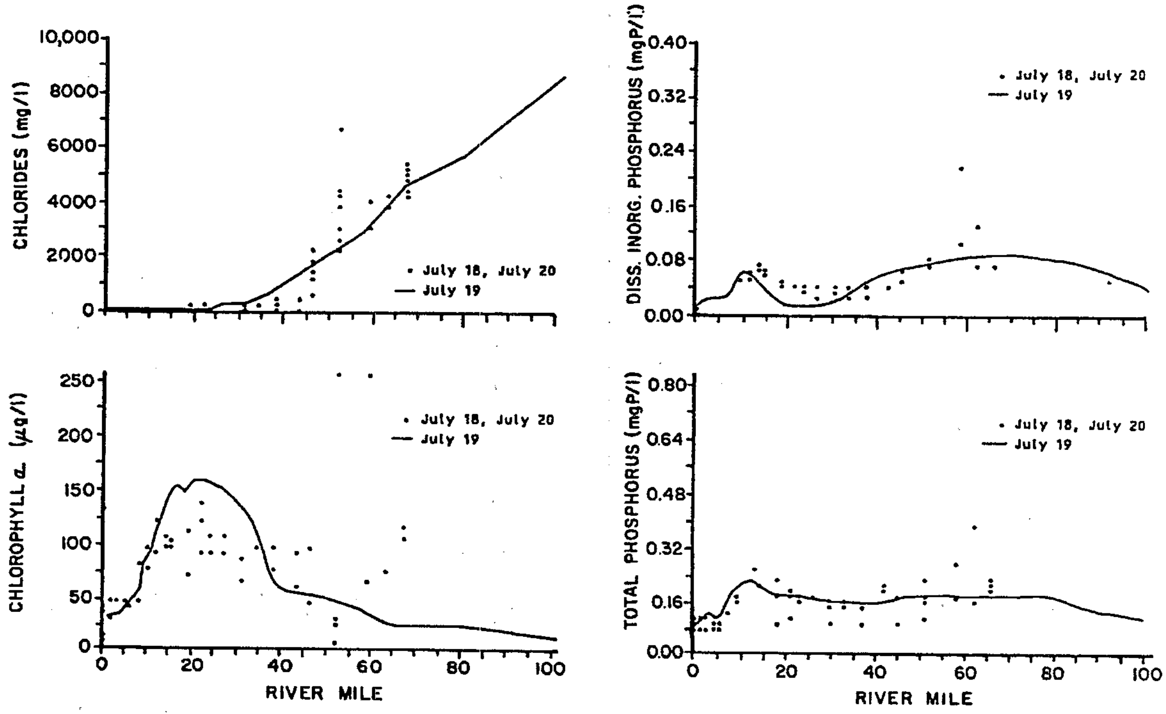

Figure 11-11. PEM verification for chlorides (mg/L), chlorophyll-a (ug/l), dissolved inorganic phosphorus (mg P/L) and total phosphorus (mg P/L), July 1977 [Hydroqual (1982)].

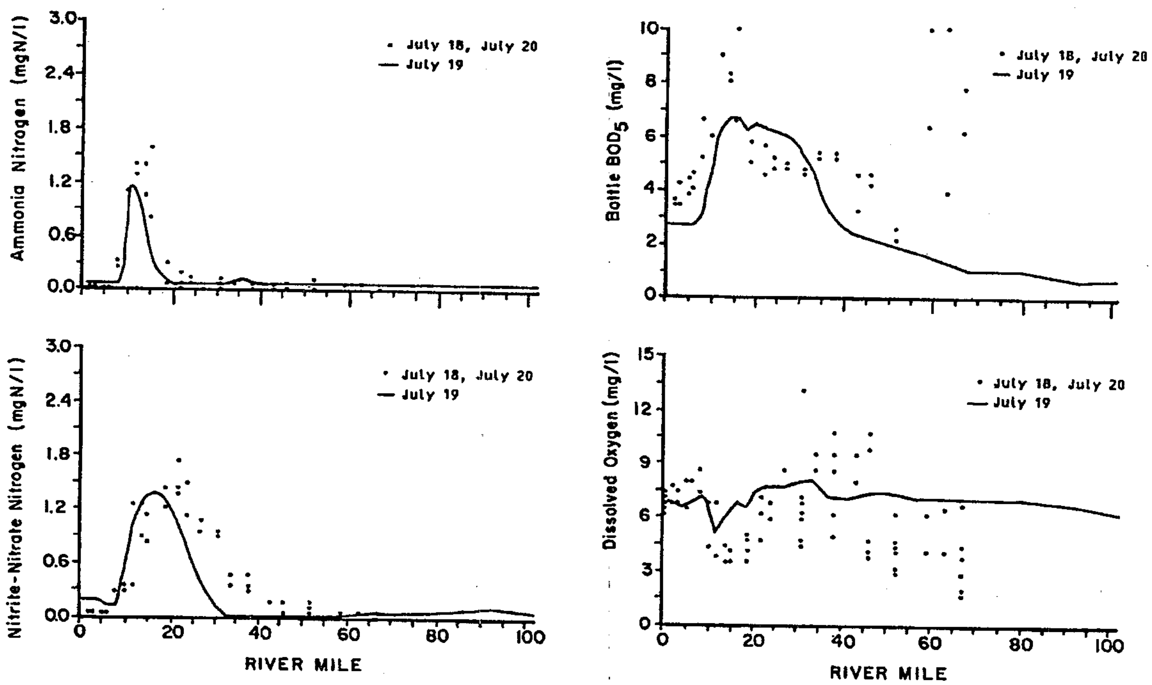

Figure 11-12. PEM verification for ammonia nitrogen (mg N/L), nitrite-nitrate nitrogen (mg N/L), bottle BOD_5 (mg/L) and dissolved oxygen (mg/L), July 1977 [Hydroqual (1982)].

Table 11-1. Linear Regression Statistics

Chlorophyll a

Year	r^2	Standard Error ($\mu g/l$)	Slope	Intercept ($\mu g/l$)	Hypothesis
1968	0.81	10.8	0.79	7.7	R
1969	0.75	10.8	0.76	2.5	R
1977	0.73	17.6	0.84	12.99	A
1978	0.88	4.3	0.70	12.26	R
1979	0.78	2.3	0.35	20.00	R

Dissolved Oxygen

Year	r^2	Standard Error (mg/l)	Slope	Intercept (mg/l)	Hypothesis
1968	0.60	0.74	0.83	1.55	A
1969	0.93	0.38	1.16	-0.76	A
1970	0.74	1.41	0.58	2.45	R
1977	0.73	0.93	1.21	-1.12	A
1978	0.75	0.59	0.68	2.77	R
1979	0.68	0.56	1.08	-0.29	A

The relative errors of the summer average means of the principal state variables were also calculated in the PEM study. These values indicate a large degree of variation among variables for any one year, as well as across years for any one variable. The median relative errors, ranged from 10 to 30 percent for chlorophyll a, 5 to 10 percent for DO, and 15 to 25 percent across all variables.

In comparing the means, a Student's "t" test was used to determine the difference between the observed mean and the computed mean. If there was no significant statistical difference between the means, the model was assumed to be verified. This statistic indicates that there was no statistical difference between observed and computed summer means for 77 percent of the variable-segment pairs for which a comparison could be made.

11.4.8. Post-Audit

Despite the continued reduction in point source phosphorus loading and gradual improvement in water quality, a massive and unexpected bloom of blue-green algae occurred in the Upper Potomac during the summer of 1983. By August, the bloom had exceeded 200 $\mu g/l$ of chlorophyll *a*. The bloom continued into the months of September and October. The occurrence of the 1983 algal bloom offered a unique opportunity to evaluate the predictive capability of PEM. A post-audit PEM simulation was performed to test the ability of the model to predict the observed bloom conditions (Hydroqual, 1989).

The PEM post-audit was conducted in conjunction with an Expert Panel convened to investigate the cause of the bloom. Their conclusions (Thomann et al, 1985) can be summarized as follows:

- PEM was able to successfully predict chlorophyll concentrations in the portions of the estuary upstream of the bloom, and was able to predict the onset of the bloom to nuisance levels through the end of July.
- PEM was not able to predict the intensification of the bloom, neither in magnitude nor spatial or temporal extent.
- Model comparison to data indicated that there was a significant source of phosphorus to the bloom area that was not being considered by PEM.

The Expert Panel subsequently recommended that investigations be undertaken to define the source of increased nutrients. These investigations were to include evaluation of pH effects on sediment nutrient release, and evaluation of the factors controlling alkalinity and pH in the Potomac. The Expert Panel also recommended that PEM be updated to include newly identified factors.

The first revision of PEM incorporated the results of bloom-related experiments that indicated increases in water column pH could significantly increase the magnitude of sediment nutrient flux. This resulted in the addition of two components to PEM: 1) simulation of pH, and 2) inclusion of a pH-mediated sediment flux. The simulation of pH required the addition of a separate submodel to simulate the equilibria between the multiple forms of inorganic carbon. This pH-driven equilibrium is also affected by algal photosynthesis, which increases water column pH. The second submodel added to PEM related to pH-mediated sediment release. The original version of PEM simulated sediment quality and the flux of nutrients across the sediment water interface. The updated PEM removed these sediment computations and replaced the predicted nutrient flux as a pH driven boundary condition.

This "first revision" of PEM provided improved prediction of 1983 conditions over the original version, but was still unsatisfactory for the relationship between phytoplankton, dissolved oxygen, nutrients, and the carbonate system. PEM was then further updated to include a second algal species representative of the blue-green alga *Microcystis,* which was the primary component of the observed bloom. Re-calibration of the model provided an improved description of the observed data.

11.5. Finite Element Model

Chlorine has been used extensively as a wastewater disinfectant and as an agent to prevent biofouling in cooling waters. Concerns have been raised that the discharge of chlorine in wastewater to the Upper Potomac Estuary might pose ecological health risks. In particular, discharges from opposing shorelines might result in a cross channel barrier that could prevent fish movement and migration. This study was conducted to determine the occurrence and fate of residual chlorine in the Potomac and to evaluate the likelihood of the formation of a toxic cross channel barrier.

A comprehensive study was conducted involving field surveys of discharge and Potomac Estuary total residual chlorine (TRC) concentrations. The objectives of the study were to document the current spatial extent of TRC; to develop and calibrate a two dimensional TRC model for testing various environmental scenarios; and to conduct model analysis of the various scenarios to establish the risk of a chlorine barrier.

The study area of the Potomac Estuary is freshwater but hydraulically influenced by ocean tides. The confluence with the Anacostia River, numerous embayments, and highly variable channel physiography make this section of the Potomac Estuary hydrodynamically complex. The data available to support a TRC model were limited to grab samples in only the longitudinal and lateral dimensions. Modeling was therefore constrained to two dimensions. This was, however, consistent with the purpose of the modeling — to define the lateral and longitudinal extent of effluent residual chlorine plumes as a potential barrier to fish migration.

The complex physiography of the upper Potomac Estuary did not allow use of simple analytical models. One-dimensional water quality models were of little use for evaluating the chloride discharges because the lateral extent of contamination could not be simulated. Branching one-dimensional estuary models, such as the Dynamic Estuary Model (DEM) may be configured to run as pseudo-two-dimensional models but have unrealistically high dispersion for localized calculations and poor characterization of two-dimensional transport. For these reasons, a true two-dimensional hydrodynamic and water quality model was required.

The Neleus chlorine model selected for this study consists of a hydrodynamic model linked to a water quality model. The hydrodynamic model solves the complete non-linear, two-dimensional, partial differential equations of fluid motion (Katopodes, 1987; LTI, 1987). The equations are integrated over time using a modified Petrov-Galerkin finite element model numerical technique yielding surface elevation and velocity at each of the model grid nodes. The results are input as mass transport terms to the water quality model.

The water quality model uses the same grid framework as the hydrodynamic model and is represented by a two-dimensional, vertically averaged, partial differential equation of mass transport. The equation includes terms for advective and diffusive mass transfer, mass sources and/or sinks, and first-order decay. The numerical solution is obtained in the same manner as with the flow equations except that an iterative solution is not required since the mass transport equation becomes linear with the assumption of zero diffusive flux at the model boundaries.

11.5.1. Model Inputs

The Neleus model required a finite element grid comprising 1171 quadrilateral elements with 1408 nodes (element intersections) as shown in Figure 11-13. This fine detail was required because of complex bathymetry. In addition, grid resolution had to be high near pollutant sources to maintain numerical stability during computation and to provide accurate model predictions within fairly short distances of discharge locations.

After setting the model grid, model inputs for boundary conditions and loadings were determined. These included tidal elevation and flows. The NOAA Tide Tables provided minimum and maximum tidal elevations and a sinusoidal interpolation scheme was used to provide tidal elevations for each hydrodynamic model time step. Some actual recorded tidal elevation data were available for use in modeling the residual chlorine surveys. Minimum and maximum elevations and time (NOAA, 1984) were abstracted from the continuous record. Advective freshwater discharges were specified as nodal velocities at the upstream ends of the model for each simulation. These were determined using information from USGS flow records for both the Potomac (at Chain Bridge) and Anacostia channels.

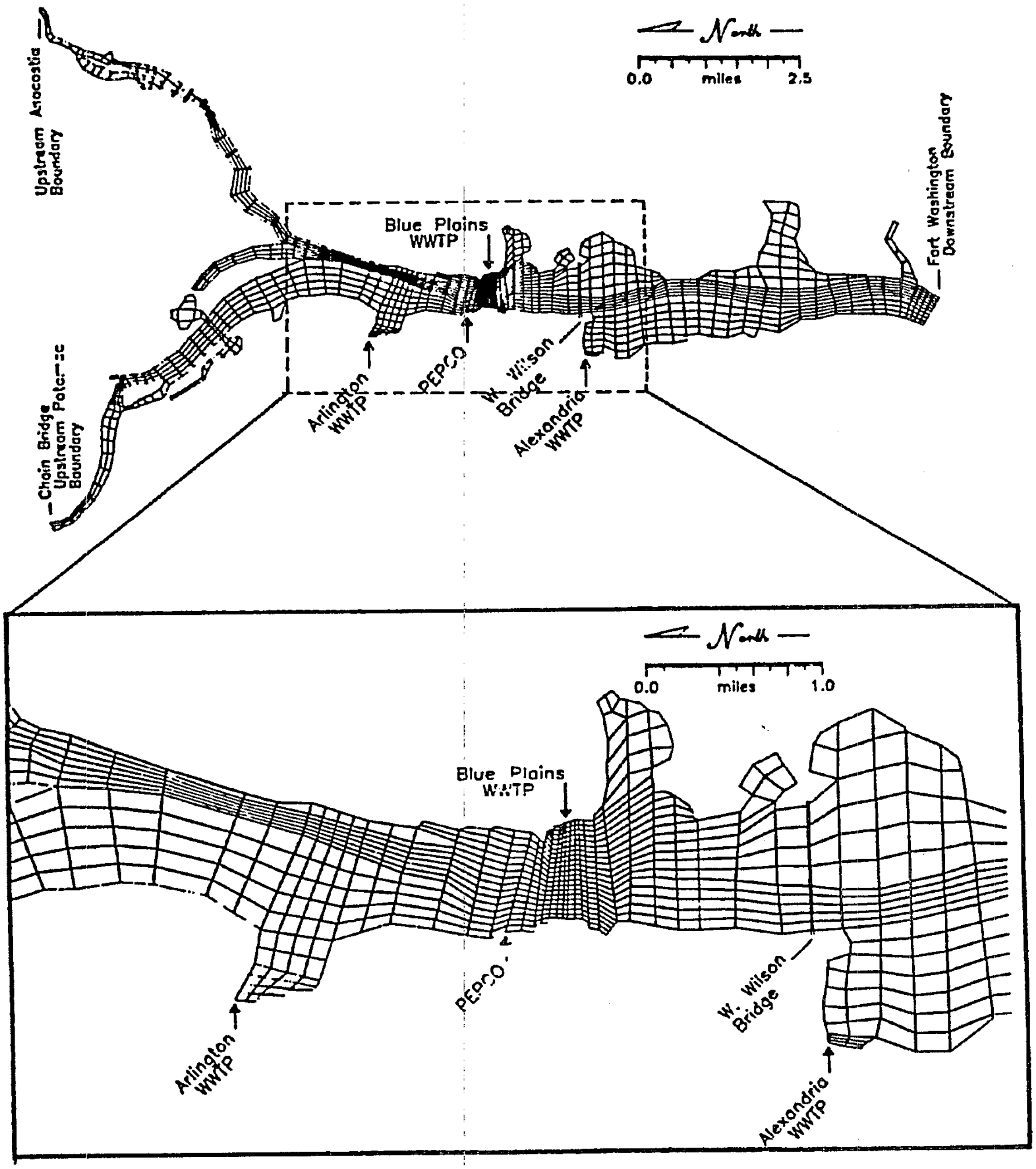

Figure 11-13. Chlorine model finite element grid network [LTI (1987)].

Daily variations in discharge were incorporated in simulations when appropriate.

In terms of pollutant inputs, four chlorine discharge locations were identified in the study area as:

- Blue Plains WWTP
- Alexandria WWTP
- Arlington WWTP
- PEPCO Power Plant

The Blue Plains Wastewater Treatment Plant was the only source for which information was known about outfall configuration and precise location. As a result, the other chlorine sources were treated as mass pollutant loadings with no momentum effects. The impact of this simplification on main channel model results was minimal since Arlington and Alexandria discharge to embayments and PEPCO discharges chlorine intermittently at very low levels.

11.5.2. Available Data

Four surveys conducted prior to the modeling effort were available for model calibration. First, the USGS conducted a dye survey over a six day period in August, 1980 (Hearn, 1984). Dye was injected for one tidal day (24.8 hours) from the Blue Plains outfall and subsequently measured throughout the study area. Three surveys conducted by the District of Columbia Department of Consumer and Regulatory Affairs provided effluent and ambient TRC concentrations throughout the tidal cycle.

11.5.3. Model Calibration/Verification

The Neleus model involved validation for both hydrodynamic and water quality models. The hydrodynamic model has one calibration parameter – Manning's n, which reflects the hydrodynamic effects of bottom roughness. The lack of hydrodynamic field data limited the calibration of the hydrodynamic model. However, previous work by Katopodes (1987) resulted in a limited calibration of the model hydrodynamics through comparison with DEM hydrodynamic predictions. A constant Manning coefficient of 0.026 was used by Katopodes (1987) and was chosen for use in the chlorine study. The water quality model has three parameters that require calibration: longitudinal and lateral dispersion coefficient, and the first-order chlorine decay rate. The dispersion terms were adjusted through simulation of the August 1980 USGS dye study, while the chlorine decay rate was selected through simulation of two of the 1984 chlorine field studies.

The 1980 USGS dye study was used to calibrate the lateral and longitudinal dispersion coefficients. The model simulation began on the 10th of August with the dye release simulation starting on the 11th. Discharge from the Blue Plains outfall was constant with a flow of 517 cfs (334 MGD) and dye concentration was 0.03446 mg/l over the release period of 24.8 hours.

Longitudinal and lateral dispersion coefficients were first estimated from literature information (Fischer et al., 1979 and McDowell and O'Connor, 1977), but refined to values of 120 ft^2/sec for longitudinal dispersion and 10 ft^2/sec for lateral dispersion. Figure 11-14 presents the model dye predictions compared to measured dye concentrations for two survey stations. These simulations assumed no decay of dye.

The model predictions follow the trends in the dye data for all stations. Evidence of dye loss is seen for stations B and C beginning on approximately August 13th. The inclusion of dye decay would improve the fit of the model to dye data, but would not affect the calibration of the dispersion terms. Since dye decay was not important to the modeling of TRC, no further model refinement for simulation of dye was performed.

The July, 1984 survey was selected for initial chlorine modeling because the sampling covered a longer time period than the other surveys. Data were collected during both day and night. The effects of daytime photolysis on chlorine decay could then be analyzed by comparing day versus night results.

Loading during the survey included a total residual chlorine concentration in the Blue Plains effluent of 0.333 mg/l at 330 MGD, in the Arlington WWTP effluent of 1.9 mg/l at 26 MGD, and the Alexandria wastewater treatment facility produced a total residual chlorine level of 1.9 mg/l at a discharge rate of 43 MGD. The PEPCO discharge was 401 MGD with intermittent effluent chlorine levels. The exact times during which chlorination occurred were not known, but the levels of chlorine applied to the cooling water were low. A constant residual chlorine concentration of 0.02 mg/l was used to represent the likely level of discharge from PEPCO.

For initial simulations, a chlorine decay rate of 12.8 per day was determined experimentally. A more conservative decay rate of 6.4 per day was also tested. The comparison of model versus data is shown in Figures 11-15 and 11-16 for averaged field data and model predictions. Averaging was used to simplify the presentation of results and because the field data were not sufficient to justify detailed comparisons. Contour lines of constant concentration are used to depict model output whereas field data are shown as singular numeric values. In general, measured chlorine levels at most field stations were too near detection limits to be considered accurate except as order of magnitude estimates. Therefore, the averaging represents the plume character well.

The comparisons of model to TRC data were considered reasonable for both loss rates. The differences in the simulations were not dramatic and and indicated that physical transport was dominant. The model characterized the dissipation of TRC especially when considering the data can only be best relied on as an order of magnitude indicator. The value of 96 μg/l just to the north of Blue Plains represents only one observation, and appears to be an anomaly. Further sensitivity analyses suggest that the lower decay rate of 6.4/day might be more representative of night time conditions, while the higher rate of 12.8/day may be appropriate for daytime.

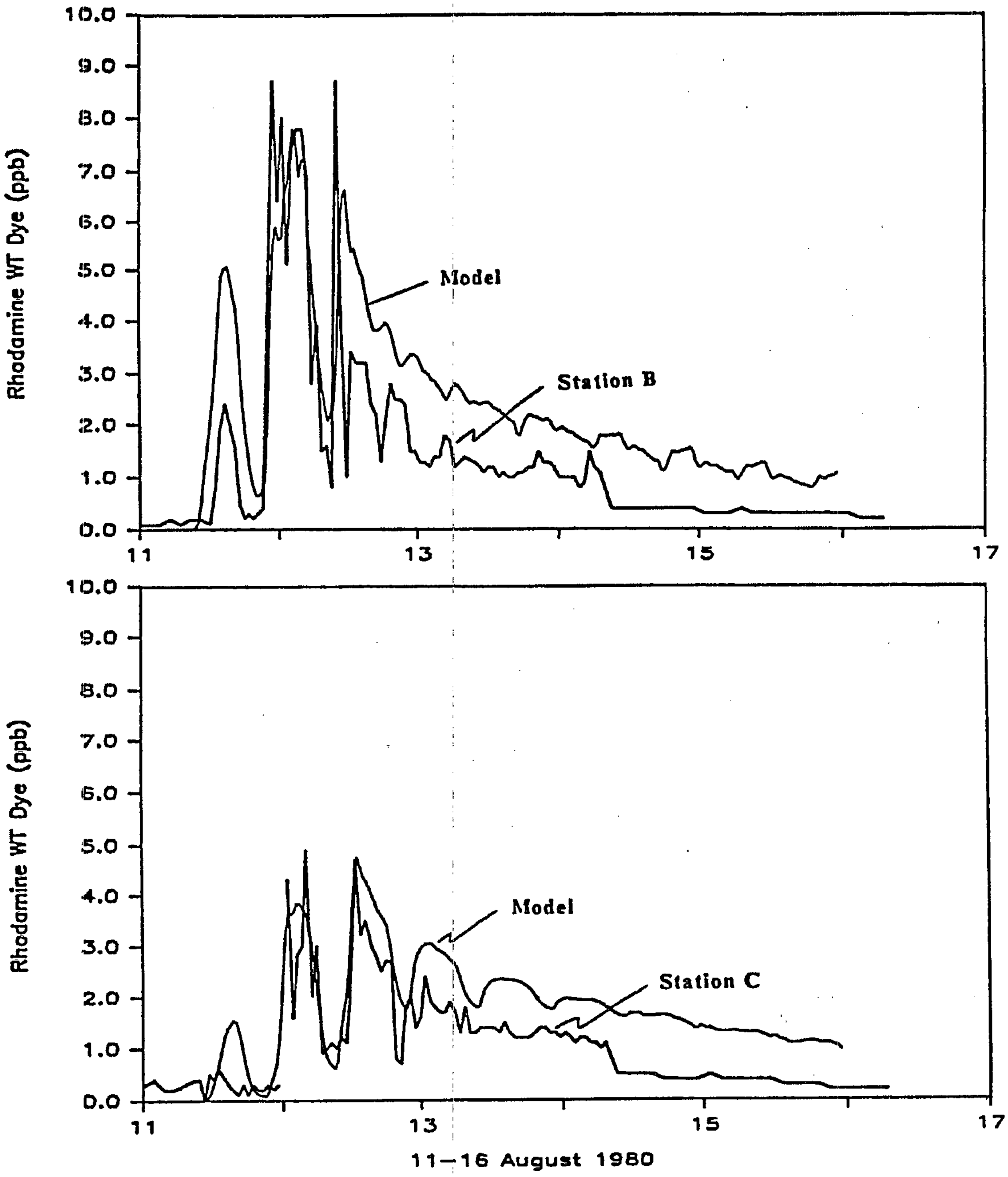

Figure 11-14. August 1980 dye survey calibration at stations B and C [LTI (1987)].

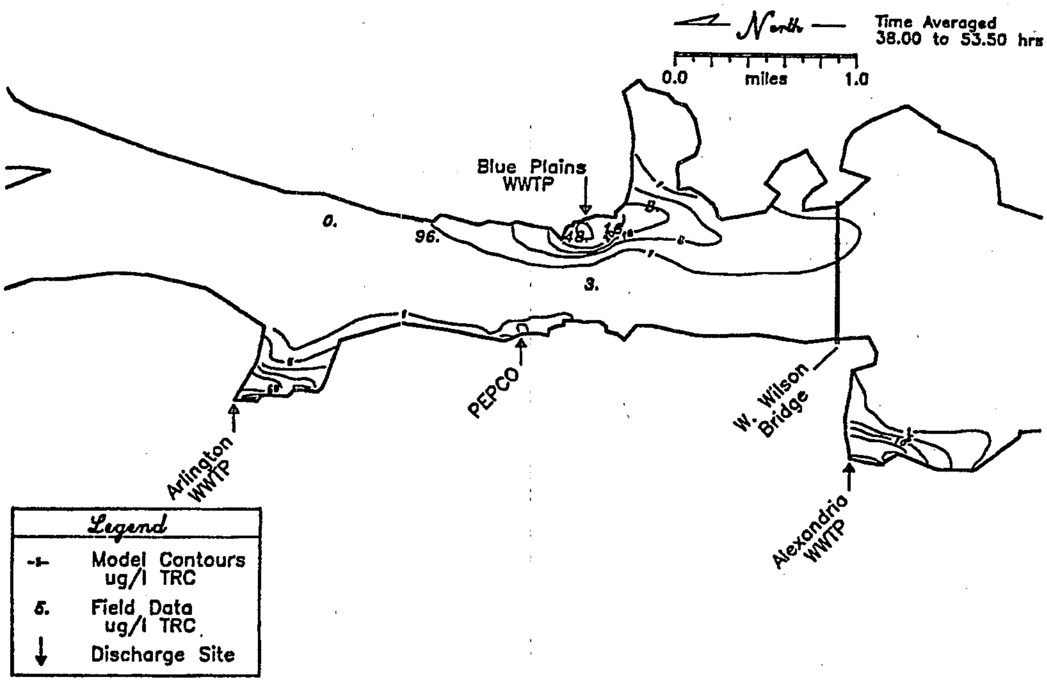

Figure 11-15. July 11, 1984 TRC survey calibration at 12.8/day loss rate [LTI (1987)].

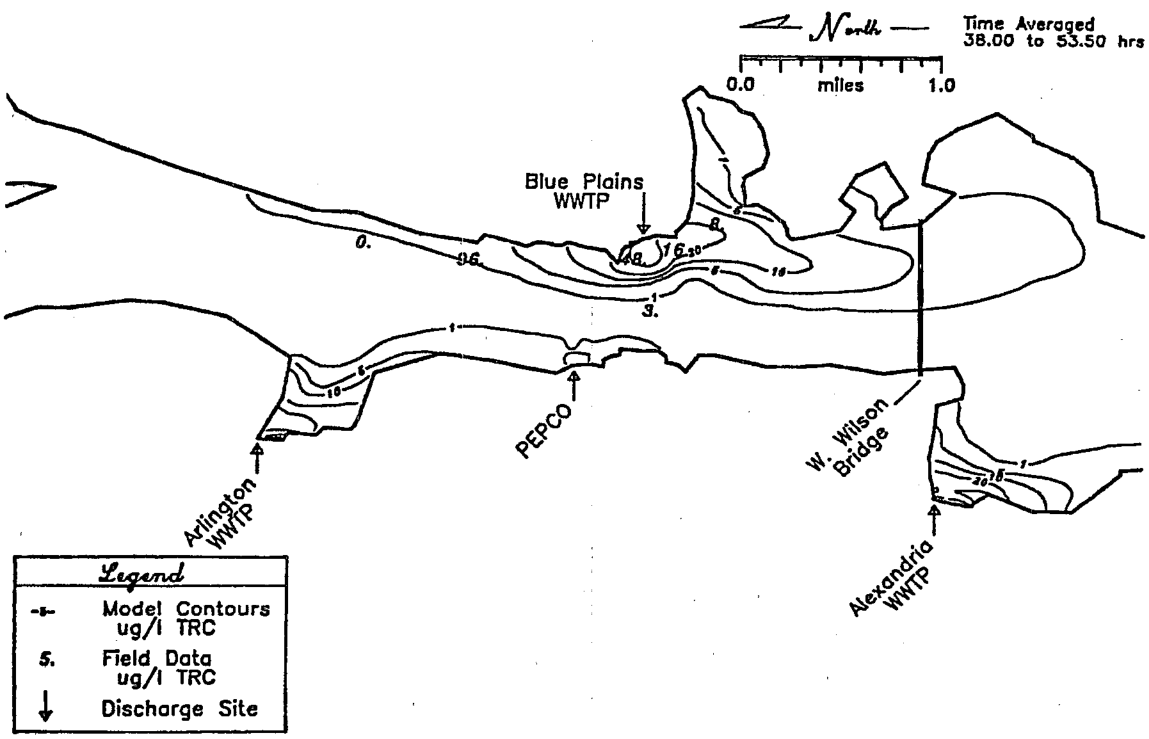

Figure 11-16. July 11, 1984 TRC survey calibration at 6.4/day loss rate [LTI (1987)].

The October, 1984 survey was chosen for model validation because it had the greatest spatial quantity of chlorine data. The dispersion and chlorine decay rates adopted for the July 1984 calibration runs were used for modeling of this survey, but inputs for actual observed loadings and ambient environmental conditions were used.

The chlorine model predictions for this survey did not compare well at certain stations but the predicted plume front and general decrease in chlorine levels moving away from the Blue Plains outfall compared well with data. As a result, the model was considered sufficiently validated to evaluate the potential for a cross channel barrier. Refined model calibration of the chlorine loss rate was not possible because of data limitations and variability. The model was still deemed well suited to assess the presence or absence of a cross channel barrier. The more conservative loss rate was used for this purpose. The modeling effort was not considered to be well suited for highly precise predictions or for waste load allocations.

11.5.4. Model Application

The potential existence of a chlorine concentration barrier was examined by model simulation over a range of conditions. These included variations in effluent loads, river flow, and tidal conditions. All other aspects of the model were identical to those used in the calibration procedure. Effluent loads to the Upper Potomac Estuary included the Blue Plains wastewater facility (370 MGD) on the east shoreline, and the Alexandria (54 MGD) and Arlington (30 MGD) wastewater facilities plus the PEPCO cooling water discharge (350 MGD) on the Western shoreline. The discharge values for the wastewater treatment facilities represent estimated capacity needs for the period 2005-2010 (MWWRPB, 1986). The Arlington and Alexandria discharges were examined at a 1.0 mg/l total residual chlorine (TRC) concentration. The PEPCO chlorine discharge level used was 0.02 mg/l. Blue Plains, the largest wastewater plant was examined under two TRC scenarios, 0.02 mg/l and 0.40 mg/l TRC. This represented conditions with and without dechlorination.

Three Potomac river flow conditions were examined. The critical seven day, ten year drought low flow (7Q10) of 470 cfs, and two April flow conditions to characterize a period of likely fish migration. The long term average April flow (19,900 cfs) was simulated as well as the lowest recorded mean monthly April flow (7,573 cfs). For the three conditions the actual corresponding Anacostia River flows were 8, 165, and 345 cfs, respectively.

Model results for the various simulations are summarized in Figures 11-17 to 11-19. For each simulation, model results were examined for all phases of the tide: ebb, flood, and slack. For these purposes, the model output has been displayed for the most critical condition where the chlorine residual extends the furthest distance across the Potomac. Model results for other periods in the tidal cycle were less critical and are not shown. A 10 μg/l criterion for TRC was used to characterize the plume boundary because this is the District of Columbia water quality standard. The figures display the boundaries of the 10 and 2 μg/l TRC concentration contours. Higher concentrations were only apparent in the immediate vicinity of the discharge pipes and dissipated quickly. These very near zone discriminations were not a model objective, and cannot be examined accurately by this model. A jet plume model that incorporates the hydraulic characteristics of the the discharge itself would be required to evaluate water quality impacts in the immediate vicinity of the discharge.

Among all examined scenarios, no conditions were simulated where the 10 μg/l concentration boundary extended across the entire Potomac and presented a potential TRC barrier. At the 0.4 mg/l level of TRC in Blue Plains effluent, the boundary extends approximately one third of the river width. Discharges from Alexandria and Arlington were largely dissipated in their respective embayments. The PEPCO discharge only minimally impacted the main channel. For 0.02 mg/l TRC (dechlorination) at Blue Plains, the plume is barely observable in the main channel. All predicted main channel concentrations were less than 10 μg/l.

In the model calibration section of this case study, the deficiencies in the calibration data sets were noted, as was their significance to model uncertainty. Nonetheless, the uncertainty in model rates would not be sufficient to alter the basic findings. Reasonable changes in dispersion rates had small effects on the plume width. In addition, for forecast purposes a conservatively low chlorine loss rate was used. This maximized the predicted plume persistence.

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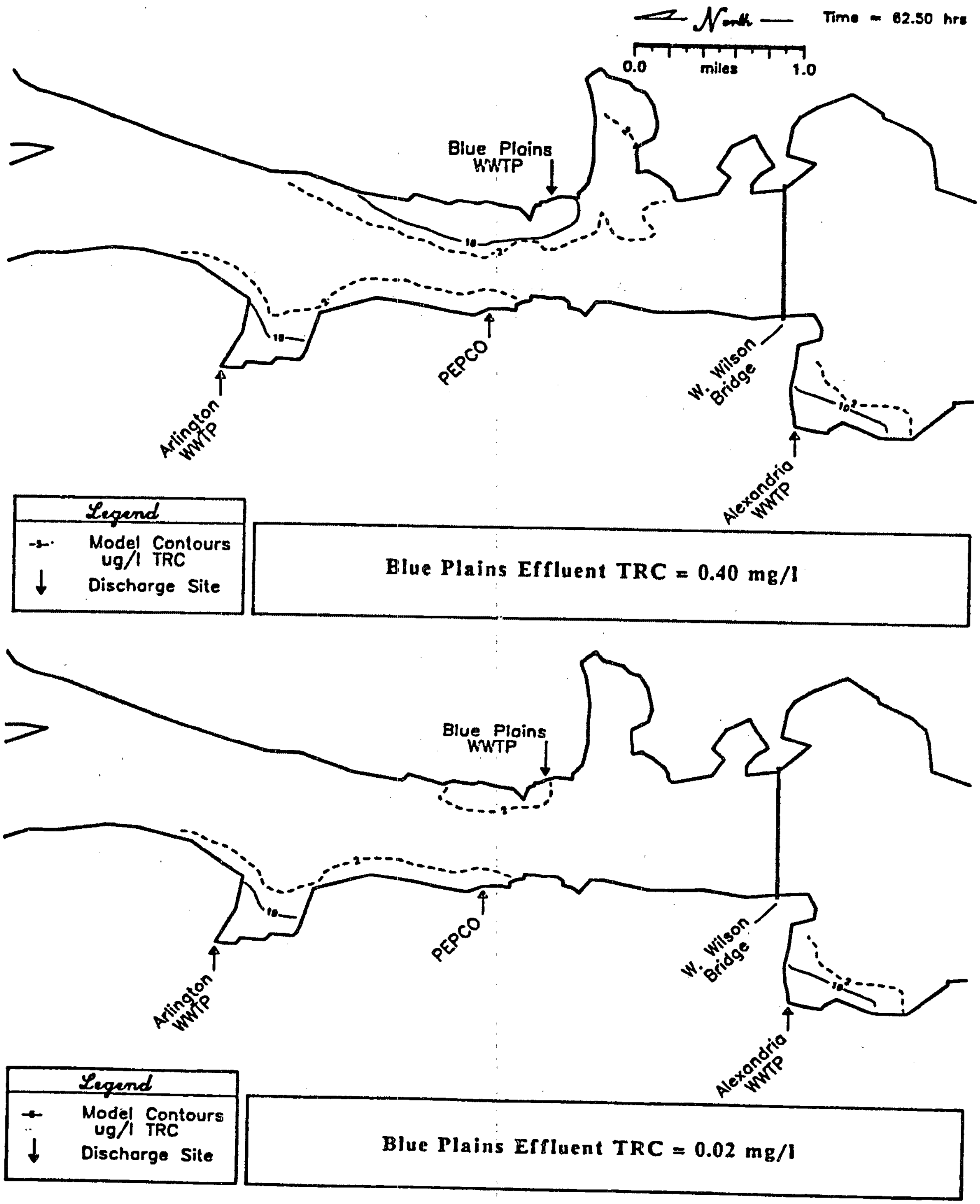

Figure 11-17. TRC model projection for 7Q10 low flow conditions [LTI (1987)].

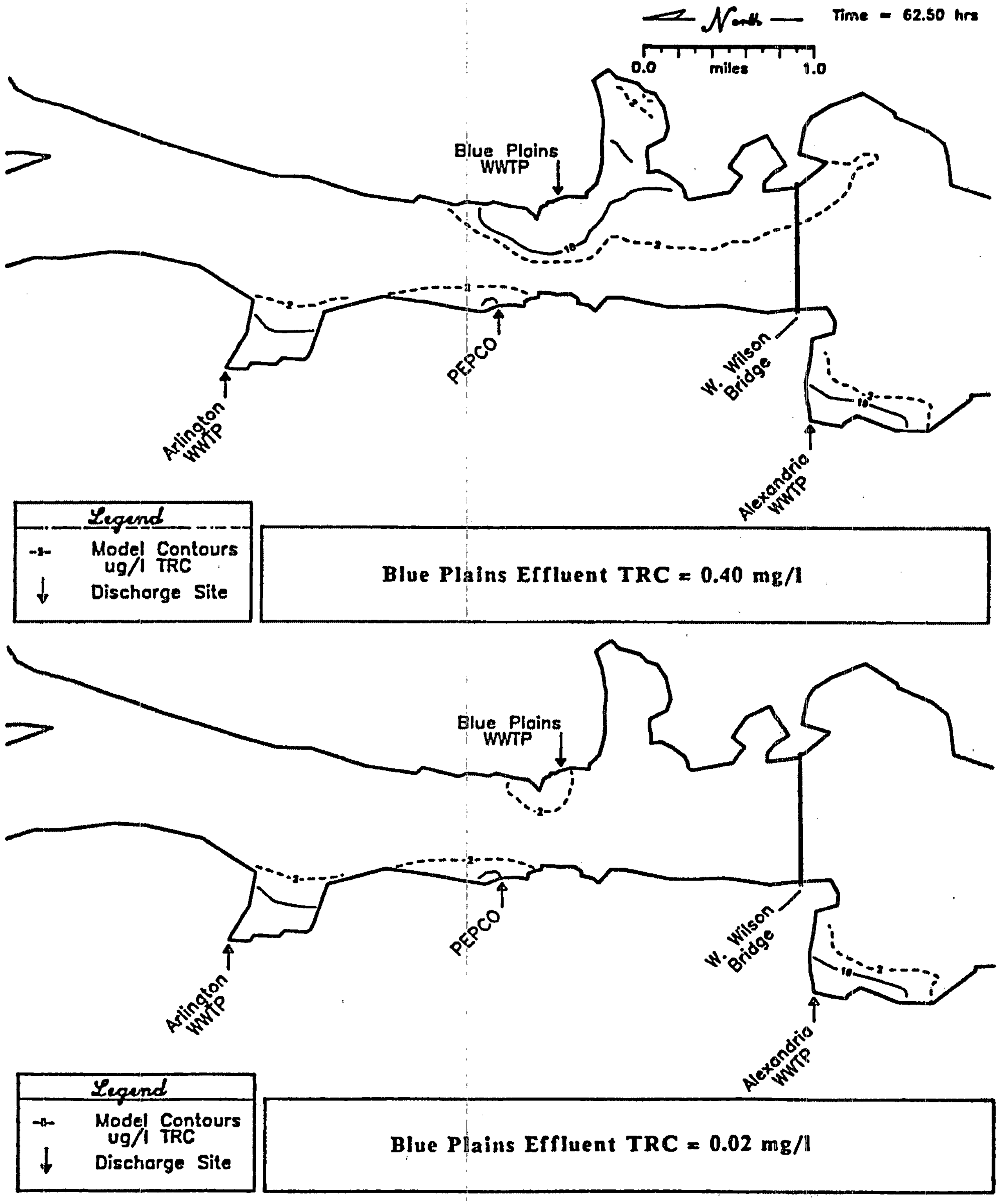

Figure 11-18. TRC model projection for average April flow conditions [LTI (1987)].

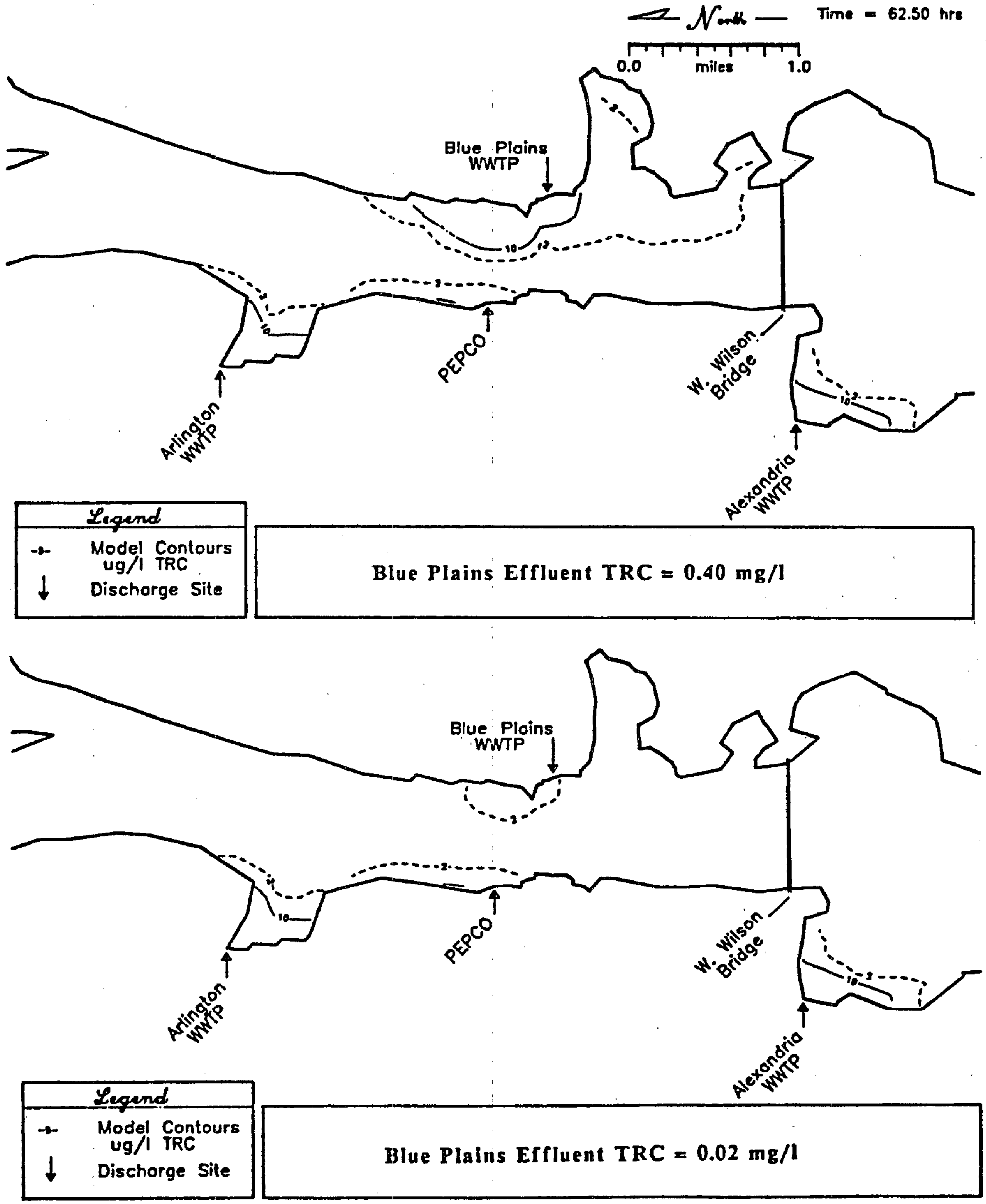

Figure 11-19. TRC model projection for lowest April flow conditions [LTI (1987)].

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12. Manasquan Estuary Real Time Modeling

12.1. Background

This study of the MIT-Dynamic Network Model (MIT-DNM) demonstrates the successful calibration and verification of a real-time estuary model. Unlike tidally-averaged or steady-state models, real time models simulate changes in flow and water quality constituents on an hour to hour basis. MIT-DNM was selected by the Manasquan River Regional Sewerage Authority to predict the effect that the discharge from a proposed wastewater treatment plant would have on the water quality and ecology of the Manasquan Estuary (Najarian et al., 1981). The Authority was primarily concerned with nutrient enrichment and primary productivity in the estuary. A real time model was selected to predict photosynthesis effects on diurnal DO concentrations and investigate the transient impacts of nonpoint source pollution and salt water intrusion.

The hydrodynamic submodel of MIT-DNM uses a finite element approach to solve the one-dimensional continuity and momentum equations for unsteady flow in a variable area channel. Dispersion is defined by the degree of stratification and the non-dimensional longitudinal salinity gradient using the relationship formulated by Thatcher and Harleman (1972, 1981). The flows and velocities calculated by this submodel are used in another submodel in which a sequence of conservation of mass equations calculates the temporal and spatial variation in the water quality parameters.

The following state variables are included in this version of MIT-DNM:

- Diatoms
- Nitrite and nitrate
- Nanoplankton
- Carbonaceous BOD
- Dinoflagellates
- Dissolved Oxygen
- Organic detritus N
- Chlorides
- Ammonium - N
- Fecal coliform
- Herbivorous zooplankton

The model assumes that the dominant activity in the estuary is aerobic and that nitrogen is the only nutrient that limits the growth of algae. Water quality processes represented in the model include phytoplankton growth, mortality, and sinking; zooplankton grazing, mortality, and excretion; nitrogen cycling and fluxes at the sediment/water interface.

12.2. Problem Setting

The Manasquan Estuary is approximately 7.6 miles long, extending from the Atlantic Ocean to Brick Township in east central New Jersey. The estuary receives inflow from the Atlantic Ocean, the Manasquan River, and Barnegat Bay, which is connected to the estuary by Point Pleasant Canal. The landward reaches of the estuary are very shallow, with large embayment and marsh areas. Figure 12-1 shows the study area with sampling stations.

Flow records for this area came from USGS gage data at Squankum on the Manasquan River. The freshwater low flow was 17.0 cfs, which included 6.2 cfs from wastewater treatment plants discharging upstream of the gage. At the time of the study, no other major point sources discharged into the river or the estuary. The Manasquan River Regional Sewerage Authority, however, proposed the construction of a regional advanced wastewater treatment facility that would discharge 9.4 cfs of effluent at the head of tide of the estuary. The plant would obviously be a major contributor to the freshwater flow into the estuary under low flow conditions.

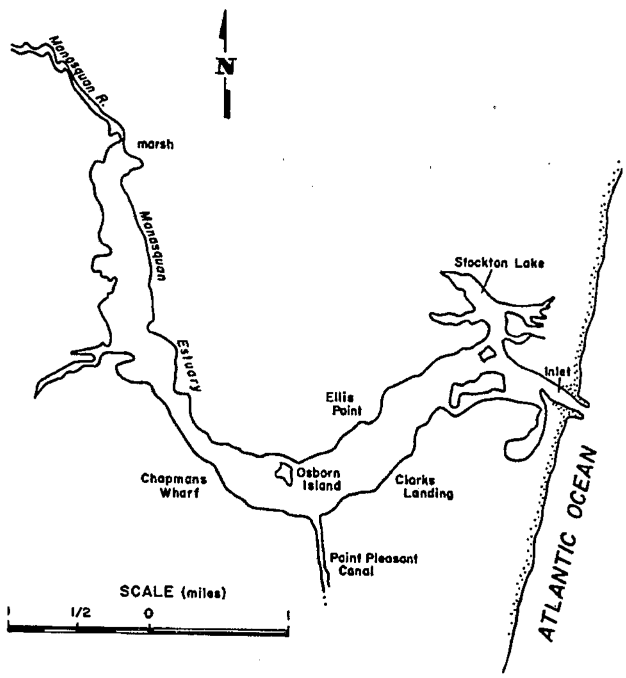

Figure 12-1. Manasquan Estuary and Inlet [Najarian et al. (1981)].

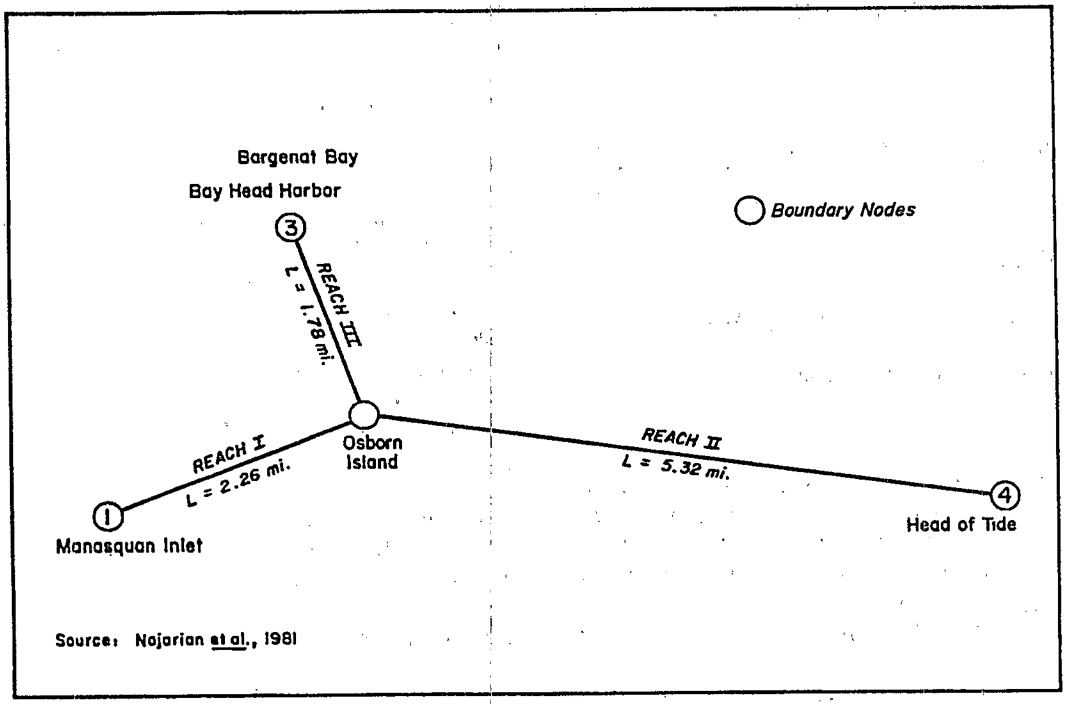

Figure 12-2. Model conceptualization of the Manasquan Estuary and the Point Pleasant Canal System [Najarian et al. (1981)].

Effluent standards to be met by the proposed plant were established by the Authority and are shown in Table 12-1.

The flow and salinity dynamics in the Manasquan Estuary system are forced by two tidal boundaries at Barnegat Bay and the Atlantic Ocean and by the freshwater inflow from the Manasquan River. Differences in tidal amplitudes and phases between the ocean and the bay cause a complex flow regime in the estuary. The tidal boundaries also differ in water quality. While the constituent concentrations at the ocean boundary are relatively constant, the concentrations at the bay boundary are much more variable due to the mixing of bay waters with Manasquan water.

Table 12.1. Effluent Quality Standards

Parameter	Standard
BOD_5	95% removal
NH_3-N	2 mg/l
DO	6 mg/l
pH	5.5-7.5
NO_3-N	7 mg/l
Cl_2	None detectable by EPA-approved methods of analysis.
Others	Such that New Jersey Surface Water Quality Standards for FW-2 Trout Maintenance Streams will be met.

Figure 12-2 shows a schematic of the MIT-DNM reach system established for the estuary. The first reach extends 2.26 miles landward from Osborn Island. The second reach extends from Osborn Island to the Atlantic Ocean, and is 5.32 miles long. The third reach, 1.78 miles long, represents Point Pleasant Canal. Each reach is represented by geometrically irregular cross-sections, with embayment volumes specified for Lake Stockton and Sawmill Creek. Tidal boundaries are specified for nodes 1 and 3, and an inflow boundary is specified at node 4.

12.3. Model Calibration

Figure 12-1 showed the location of stations for model calibration sampling performed in July and August, 1980, by Elson T. Killam Associates, Inc. Two sampling events were conducted over a four-day period — July 21-24 and August 25-28, 1980. Salinity and nutrient concentrations at each station were measured during daylight hours at frequencies of 3-4 observations per tidal cycle.

The measured water quality parameters were as follows:

- Temperature
- Dissolved Oxygen
- Salinity
- Secchi Depth
- Dissolved Org.-N
- Particulate Org.-N
- Ammonia
- Nitrite
- Nitrate
- Ortho-phosphate
- Silicate
- Chlorophylla
- BOD

The zooplankton and phytoplankton species present during each sampling event were identified. In addition, synoptic data on the tides and the freshwater inflow at the boundaries and at three instream stations in the Manasquan Estuary were also collected. Freshwater inflows at the head of the estuary in July and August persisted at about 30 to 40 cfs without any dramatic increases between the two sampling events. The August data set was selected for model calibration because all three algal species represented in the model (diatoms, nanoplankters, and dinoflagellates) were present during this month. The July data set was used for the purpose of model verification.

12.3.1. Hydrodynamic Submodel Calibration

Calibration of model hydrodynamics must precede water quality calibration. In the Manasquan study, it was imperative to start the model with realistic initial hydraulic and salinity conditions since field observations only covered a 4 day or 9 tidal cycle period of time. To establish realistic initial conditions for the August 24-28 sampling event, the model was run for an antecedent period of three tidal cycles that damped out transients resulting from unrealistic initial conditions. Repeating tides of 12.42 hour periodicity were imposed at the inlet and at the Bay Head Harbor boundaries. These tides were extracted from the tides observed during the first day of sampling. The necessary adjustment to tidal records at the Bay Head Harbor boundary was made to reflect the differences in the MSL elevation between the inlet and the head of Barnegat Bay. The surface elevations and velocities computed during the last time step of repeating tide simulation were then taken to be the initial hydraulic conditions for 12:30 p.m. on August 24, 1980.

Three sets of hydraulic boundary conditions were specified for each day of the simulation using observed data at the head of tide, the inlet, and Bay Head Harbor. The hydraulic calibration of the model was accomplished by matching the observed tidal ranges and the phases measured at Clark's Landing and Chapman's Wharf by calibrating Manning's friction coefficient. The model accurately simulated the observed hydraulics. The maximum difference in observed and computed data was approximately 7% of the tidal elevation range.

Salinity was calibrated next. Salinity observations did not begin until August 25, 1980. As done for tidal elevations, initial conditions for salinity were calculated by running the model for an antecedent period. The observed salinities at sampling stations on August 25 were averaged for that day and assumed as concentrations at these stations. Initial salinity concentrations at computational points between stations were generated by linear interpolation. At the two tidal boundary stations, the extreme observed salinities were assigned during the end of flooding flows and the model computed salinity concentrations during the ebbing flows. The model requires specification of the time it takes for the boundary salinities to reach the extreme observed salinities after the flood flows begin.

The freshwater inflow boundary condition is assumed to have a background salinity of 0.09 percent. To calibrate the mass transport of chlorides in the estuary, dispersion must be represented adequately. This requires calibration of the stratification parameter K and Taylor's dispersion multiplier m, both of which are used in the following dispersion equation:

$$E(x,t) = \frac{KdS}{dX} + mE_T$$

where,

$E(x,t)$ = Temporally and spatially varying dispersion coefficient (ft^2/sec)

S = s/s_o, where $s(x,t)$ is the spatial and temporal distribution of salinity (dimensionless)

s_o = Ocean salinity (ppm)

X = x/L (dimensionless)

L = Length of estuary to head of tide (ft)

E_T = Taylor's dispersion coefficient (ft^2/sec) $= 77\, unR_h^{5/6}$

u = $u(x,t)$ = tidal velocity (ft/sec)

n = Manning's friction coefficent

R_h = Hydraulic radius (ft)

K = Estuary dispersion parameter (ft^2/sec) $= u_oL/1000$

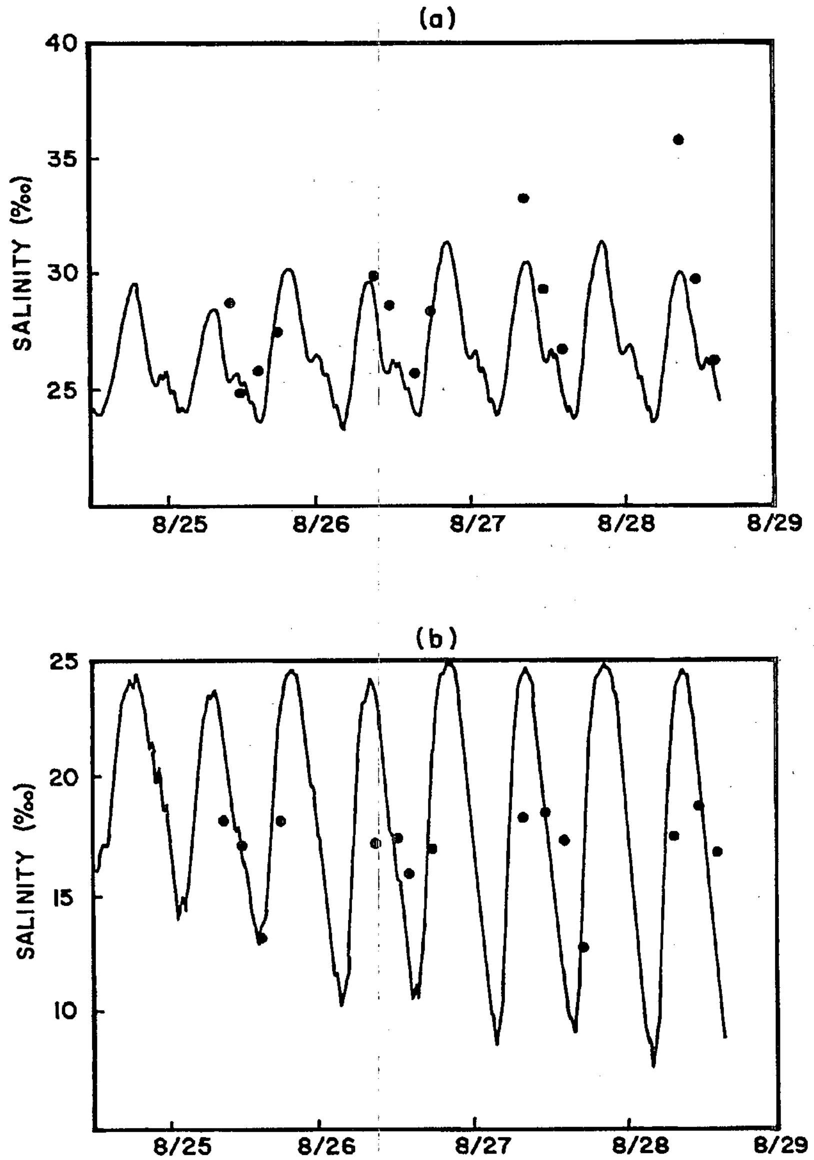

Figure 12-3. Time-varying salinity concentrations during August 24-28, 1980 at (a) Clark's Landing and (b) Chapman's Wharf [Najarian et al. (1981)].

u_o = Maximum ocean velocity at ocean entrance (ft/s)

m = Multiplying factor for bends and channel irregularities

In this case, values of K = 58.5 ft^2/sec and m = 25 were used. More information regarding the development of this equation can be found in Thatcher and Harleman (1972, 1981).

The results of the simulation of salinity concentrations at Clark's Landing and Chapman's Wharf are shown in Figure 12-3. The observed and computed salinities matched well at Clark's Landing, except for two unusually high observed ocean salinity concentrations. Because these observed values exceeded the observed ocean salinity concentrations on those days, the modelers concluded that the data points were unrealistic. Based on the plots of observed vs. simulated salinity concentration, the calculated dispersion coefficients were considered adequate.

12.3.2. Water Quality Submodel Calibration

Once the hydraulics and mass transport within the estuary were adequately defined, the model was calibrated for water quality parameters. Like the tidal elevation and salinity calibrations, this calibration required initial and boundary conditions, and also involved the evaluation of transformation rate constants based on plots of simulated versus observed data.

The system again requires the establishment of two ocean boundaries and a time-varying boundary at the head of tide, as well as initial conditions throughout the system. The ocean boundaries were handled as in the salinity calibration, where ocean concentrations were specified at the end of flood flows and water quality values were computed internally during ebb flows. Observed conditions at the Squankum USGS gage were used to define the time-varying water quality conditions at the Manasquan head of tide. Because the phytoplankton and zooplankton concentrations were sampled only once during the sampling period, time-invariant concentrations were specified at the three boundaries. Initial conditions were estimated using sampling data and linearly interpolated to establish values between sampling stations.

Unlike the hydraulics and salinity calibrations, where a combined total of three constants were calibrated on the basis of observed versus simulated data, the water quality calibration requires the determination of many constants. Table 12-2 shows the values that were established through model calibration. These are the values that best represent the site-specific kinetic processes in the Manasquan Estuary while still falling within the range of values found in the technical literature.

Examples of simulated versus observed plots for the various water quality parameters are illustrated in Figures 12-4 to 12-10. The individual symbols indicate observed data points, while the straight line shows the continuous simulation model output. These plots represent the best simulation of observed data using reasonable rate constants and coefficients. Model goodness-of-fit was determined only through visual observation of the plots; no statistical tests were performed.

Figure 12-4 shows the simulation of detritus-N, ammonium-N and nitrite + nitrate – N at Clark's Landing. The ammonium-N concentrations predicted by the calibrated model were reasonably close to observed values. The simulation of detritus-N and nitrite + nitrate-N was less accurate, particularly at Chapman's Wharf. The computed nitrite + nitrate-N concentrations were sometimes an order of magnitude lower than the observed concentrations at the station. The modelers could find no explanation for this problem. To adequately simulate detritus-N at Chapman's Wharf, a source of 240 lb/day was introduced as a distributed load. Because the estuary is very shallow, the modelers justified this input to the model by speculation that tidal disturbances could have resuspended some of the settled detritus.

The calibration of CBOD, NBOD, and DO at Clark's Landing and Chapman's Wharf are shown in Figures 12-5 to 12-10. Like the detritus-N simulation, an adequate CBOD simulation at Chapman's Wharf was not possible without the introduction of a distributed CBOD load. Even after assuming a load of 3,500 lb/day, the observed and simulated data did not match well. The DO simulation results proved to be confusing at both stations. Although low concentrations of NBOD and CBOD were observed at Clark's Landing, the observed DO levels at this station are lower than the concentrations predicted by the model. Conversely, the observed DO levels at Chapman's Wharf climbed much higher than the simulated DO concentrations, even though large CBOD and detrital nitrogen concentrations were observed there.

Because no sampling was conducted to measure phytoplankton concentrations over time, the model could not actually be calibrated for these water quality parameters. The relative proportion of each algal species was input to the model based on the observed data gathered from the single sampling event and species identification. Figures 12-11 and 12-12 show the simulated concentrations of phytoplankton nitrogen at the two stations. The plots clearly indicate a strong tidal effect upon phytoplankton concentrations.

12.3.3. Model Verification

The purpose of model calibration is to establish the values of coefficients, such as Manning's "n" or decay rates, which accurately represent the physical and biochemical nature of the system. Once these values are established, they must be verified. Using the same values to represent the estuary, the model must be applied to a different time period for which sampling data are available. If the simulated concentrations accurately predict observed concentrations the model can be considered verified.

The verification data were obtained during a sampling event in July 1980. This event, like the August 1980 sampling that provided the calibration data, was four days long, with salinity and nutrient concentrations measured during daylight hours at frequencies of 3-4 observations per tidal cycle. As in calibration, the observed data were used to establish initial and boundary

Table 12-2. Model-Governing Rate Parameters [Najarian et al. (1981)]

Transformation	Rate	Unit
K_1: Ammonification of detritus-N	0.08	day^{-1}
K_2: Diatom uptake of ammonium-N		
K_2^{opt}	0.415	day^{-1}
Y_2 (half saturation constant)	0.0122	mg-N/l
I_s (Optimum intensity of solar radiation)	144	ly/day
T_{opt} (Optimum reaction temperature)	10-15	^0C
T_{max} (Maximum temperature beyond which denaturation of cell protein occurs)	30	^0C
K_3: Nanoplankton uptake to ammonium-N		
K_3^{opt}	0.553	day^{-1}
Y_3	0.004	mg-N/l
I_s	64.8	ly/day
T_{opt}	27.5	^0C
T_{max}	30	^0C
K_4: Diatom mortality rate	0.05	day^{-1}
K_5: Nanoplankton mortality rate	0.05	day^{-1}
K_6: Copepod uptake of diatom-N		
K_6^{opt}	0.50	day^{-1}
Y_5	0.10	mg-N/A
T_{opt}	24-28	^0C
T_{max}	35	^0C
K_7: Copepod mortality rate	0.20	day^{-1}
K_8: Copepod excretion rate	0.08	day^{-1}
K_9: Nitrification rate	0.15	day^{-1}
K_{10}: Diatom uptake of (NO_2+NO_3)-N		
K_{10}^{opt}	0.376	day^{-1}
Y_4	0.0063	mg-N/l
I_s	144	ly/day
T_{opt}	10-15	^0C
T_{max}	30	^0C
K_{11}: Nanoplankton uptake of (NO_2+NO_3)-N		
K_{11}^{opt}	0.501	day^{-1}
Y_6	0.015	mg-N/l
I_s	64.8	ly/day
T_{opt}	24-28	^0C
T_{max}	30	^0C
K_{12}: Copepod uptake of detritus-N		
K_{12}^{opt}	0.34	day^{-1}
Y_1	0.250	mg-N/l
T_{opt}	24-28	^0C
T_{max}	35	^0C
K_{13}: Copepod uptake of nanoplankton-N		
K_{13}^{opt}	0.34	day^{-1}
Y_7	0.22	mg-N/l
T_{opt}	24-28	^0C
T_{max}	35	^0C
K_{14}: Dinoflagellate uptake of ammonium-N		
K_{14}^{opt}	2.075	day
Y_8	0.021	mg-N/l
I_s	288	ly/day
T_{opt}	20-25	^0C
T_{max}	32	^0C
K_{15}: Dinoflagellate uptake of $(NO_2 + NO_3)$-N		
K_{15}^{opt}	1.880	day
Y_9	0.042	mg-N/l
I_s	288	ly/day
T_{opt}	20-25	^0C
T_{max}	32	^0C
K_{16}: Copepod uptake of dinoflagellate-N		
K_{16}^{opt}	0.5	day^{-1}
Y_{10}	0.1	mg-N/l
T_{opt}	24-28	^0C
T_{max}	35	^0C
K_{17}: Dinoflagellate mortality rate		
K_{17}	0.05	day^{-1}
K_{18}: Sedimentation of detritus		
K_{18}	0.1	day^{-1}
K_{19}: Sedimentation of (NO_2+NO_3)		
K_{19}	100	ug-at $N/m^2/hr$
K_{20}: Sediment release of ammonium-N		
K_{20}	10	ug-at $N/m^2/hr$

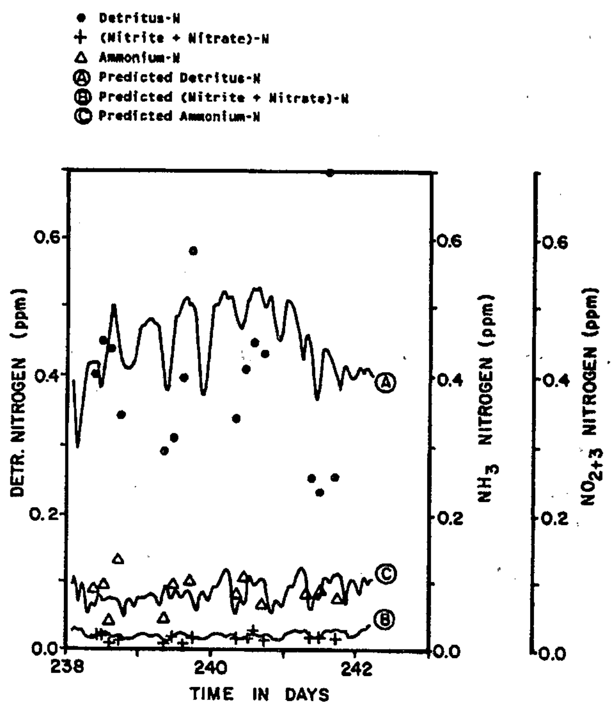

Figure 12-4. Temporal variation of Detritus-N, Ammonium-N, and Nitrite+Nitrate-N at Clark's Landing, August 25-28, 1980 [Najarian et al. (1981)].

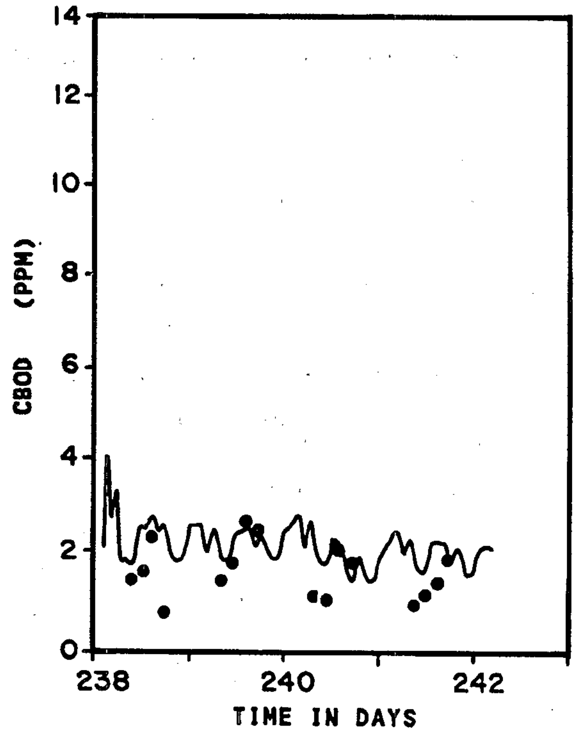

Figure 12-5. Temporal variation of CBOD at Clark's Landing, August 25-28, 1980 [Najarian et al. (1981)].

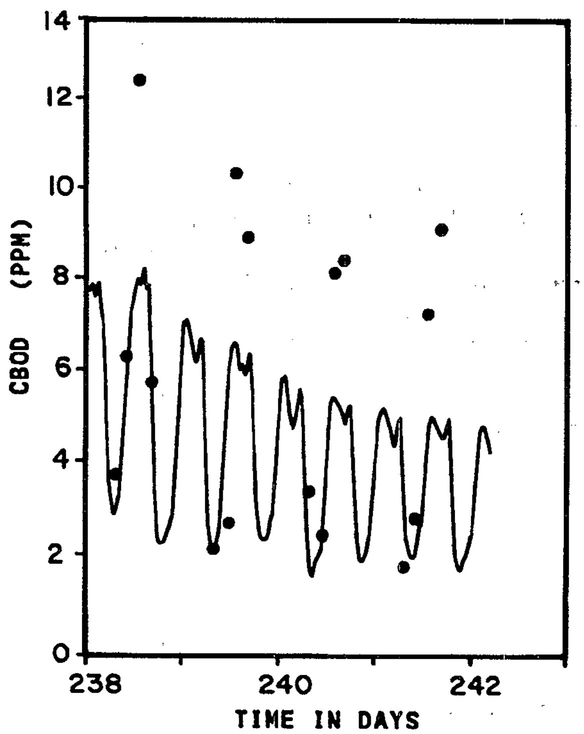

Figure 12-6. Temporal variation of CBOD at Chapman's Wharf, August 25-28, 1980 [Najarian et al. (1981)].

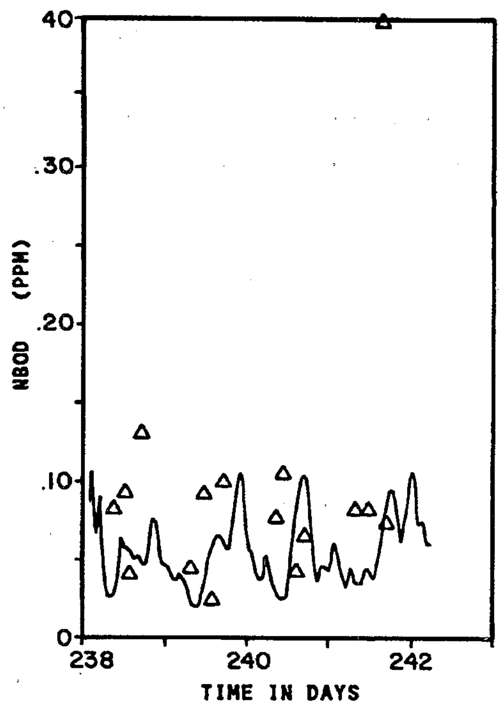

Figure 12-7. Temporal variation of NBOD at Clark's Landing, August 25-28, 1980 [Najarian et al. (1981)].

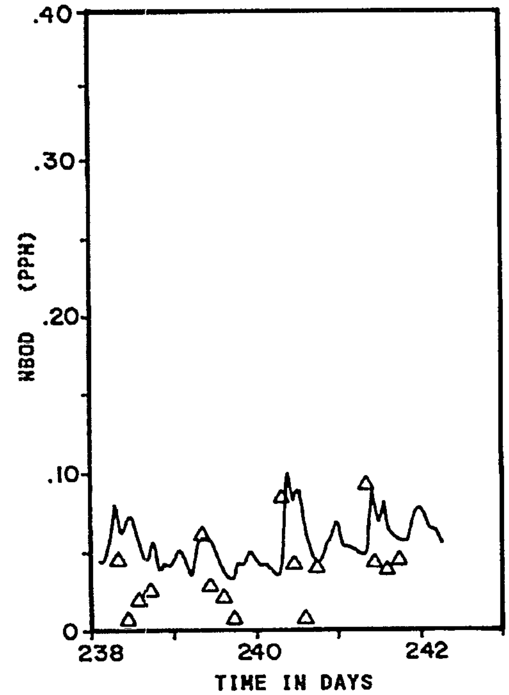

Figure 12-8. Temporal variation of NBOD at Chapman's Wharf, August 25-28, 1980 [Najarian et al. (1981)].

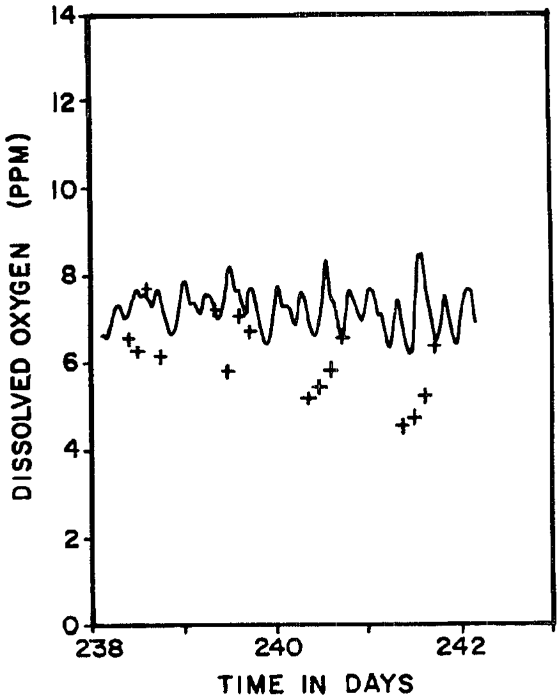

Figure 12-9. Temporal variation of DO at Clark's Landing, August 25-28, 1980 [Najarian et al. (1981)].

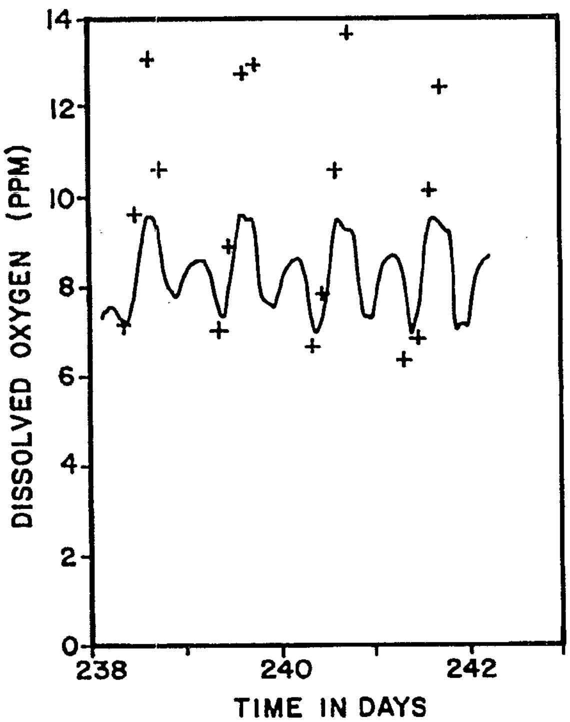

Figure 12-10. Temporal variation of DO at Chapman's Wharf, August 25-28, 1980 [Najarian et al. (1981)].

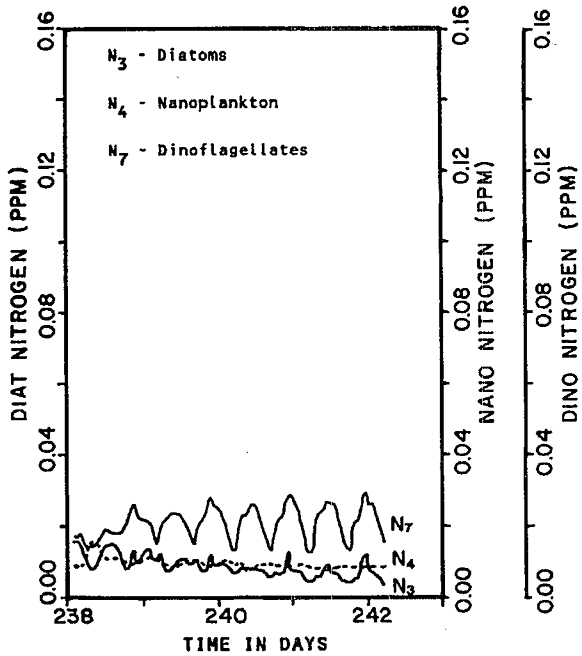

Figure 12-11. Temporal variation of Diatom-N, Nanoplankton-N, and Dinoflagellate-N at Clark's Landing, August 25-28, 1980 [Najarian et al. (1981)].

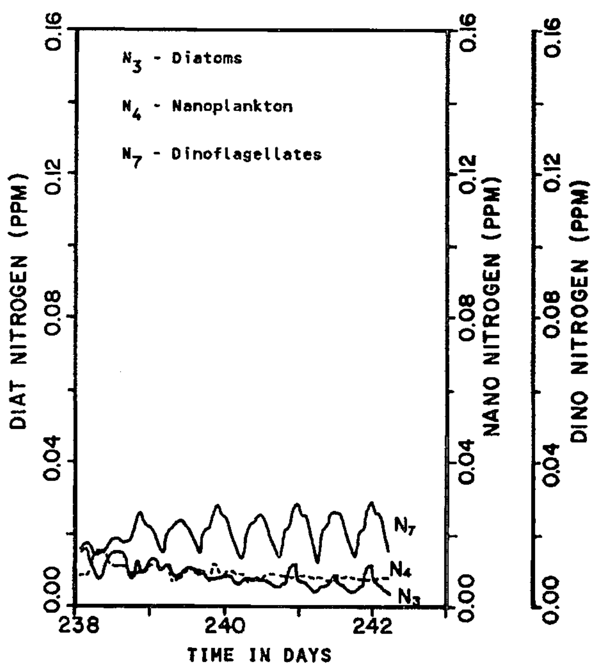

Figure 12-12. Temporal variation of Diatom-N, Nanoplankton-N, and Dinoflagellate-N at Chapman's Wharf, August 25-28, 1980 [Najarian et al. (1981)].

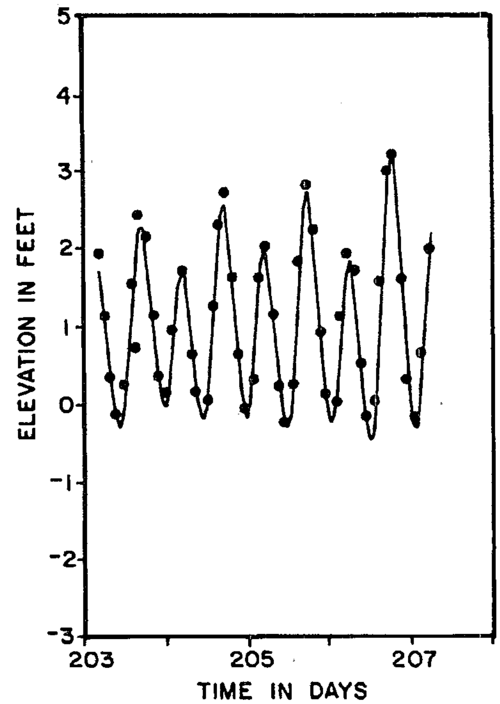

Figure 12-13. Hydraulic verification: calculated vs. observed elevations at Clark's Landing [Najarian et al. (1981)].

conditions, and to evaluate the adequacy of the simulation.

The simulation of tidal elevations was investigated first. The initial water surface elevations, the time-varying water surface elevations at the tidal boundaries, and the time-varying freshwater inflow at the head of tide were established from observed data. The Manning's "n" values, 0.018 downstream and 0.022 upstream of Chapman's Wharf, were used without change from the calibration study.

The simulation of tidal elevations at Clark's Landing and Chapman's Wharf is shown in Figures 12-13 and 12-14. The largest difference in predicted and calculated water surface elevation is approximately 0.2 feet at Clark's Landing.

The simulation of salinity was the next step in the verification procedure. The initial and boundary conditions were established in a manner consistent with the calibration study, using observed salinity concentrations at the sampling stations. The stratification parameter K and the calibration multiplier m were set equal to the values used in the calibration study. Analysis of Figures 12-15 and 12-16 show again that observed and simulated values were more similar for the verification than the calibration. The modelers were particularly pleased that the furthest inland sampling station in the estuary, Chapman's Wharf, gave the best comparison between predicted and observed values. Based on these results, they concluded that the advective and dispersive processes throughout the estuary were well represented in the model.

Finally, the model was verified for water quality processes. Again, initial and boundary conditions were established using observed data and an antecedent period simulation, and all the constants evaluated in the calibration study were used without modification in the verification study. Because of project constraints, the simulation of CBOD, NBOD, and DO was not performed. The results of the water quality comparisons are shown in Figures 12-17 and 12-18. As in the calibration study, the detritus-N concentration at Chapman's Wharf could not be accurately simulated without the specification of a distributed detrital load. The modelers found that a load of 360 lbs/day resulted in an adequate simulation; however, this load was set at 240 lbs/day in the calibration study. Because the detritus-N concentrations calculated in the calibration study were lower than the observed concentrations, the modelers concluded that the 360 lbs/day load would be valid for the calibration as well as the verification period. Other than the ammonium-N concentrations predicted at Chapman's Wharf and Osborn Island, (a station that is not included in the modeling

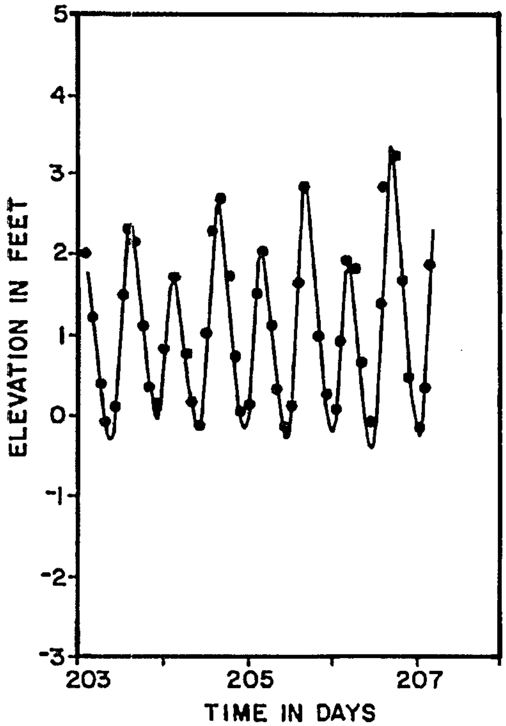

Figure 12-14. Hydraulic verification: calculated vs. observed elevations at Chapman's Wharf [Najarian et al. (1981)].

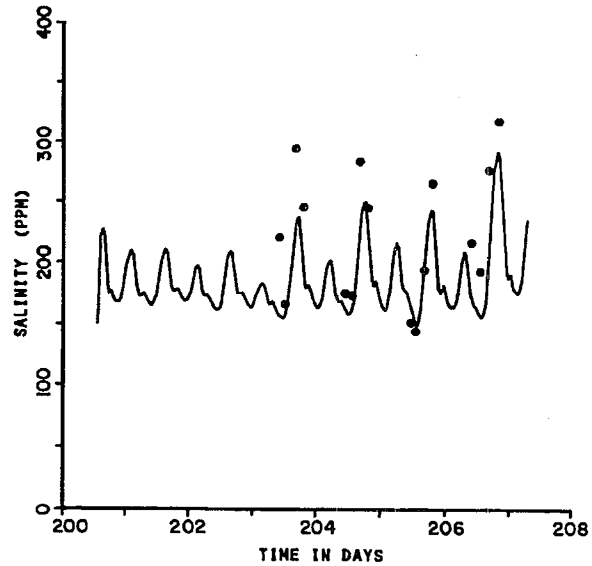

Figure 12-15. Salinity verification: calculated vs. observed salinities at Clark's Landing [Najarian et al. (1981)].

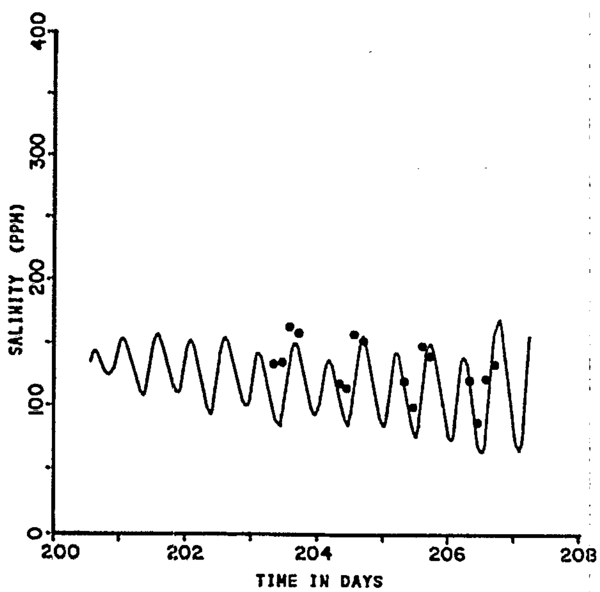

Figure 12-16. Salinity verification: calculated vs. observed salinities at Chapman's Wharf [Najarian et al. (1981)].

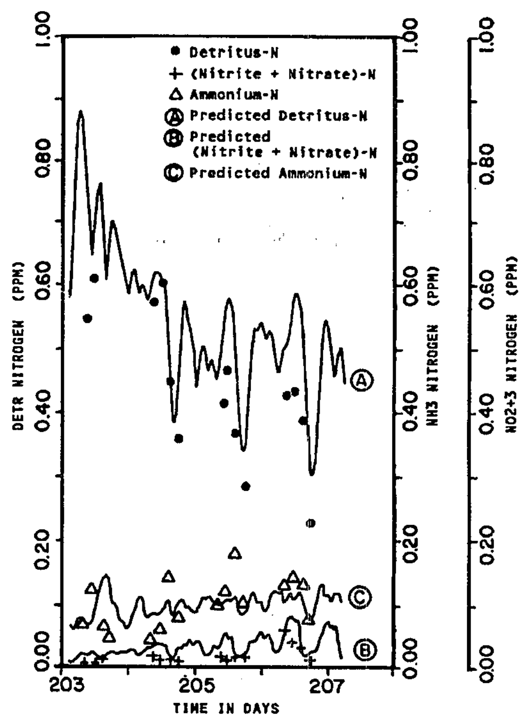

Figure 12-17. Temporal variation of Detritus-N, Ammonium-N, and Nitrite+Nitrate-N at Clark's Landing [Najarian et al. (1981)].

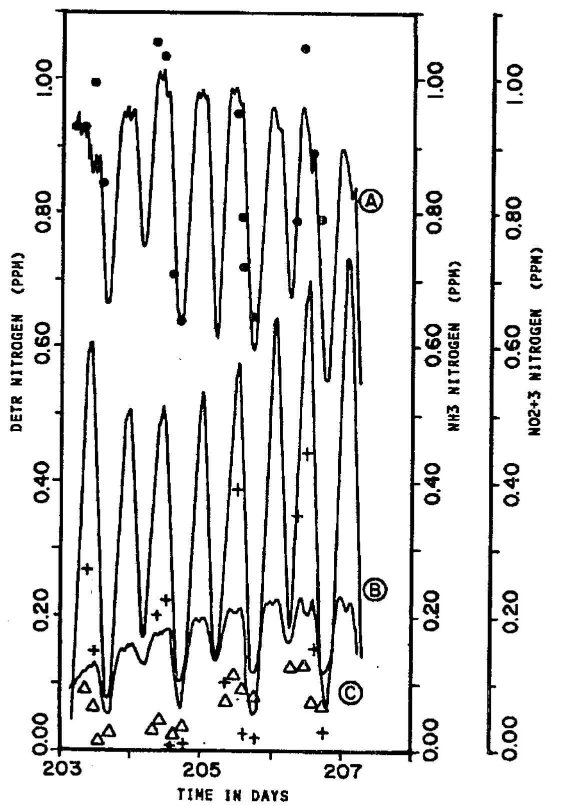

Figure 12-18. Temporal variation of Detritus-N, Ammonium-N, and Nitrite+Nitrate-N at Chapman's Wharf [Najarian et al. (1981)].

report), the water quality simulation was considered satisfactory.

12.3.4. Model Projections

The original goal of the modeling effort was to determine the impact that a proposed wastewater treatment plant effluent would have upon water quality in the Manasquan Estuary. However, the plans for the new wastewater treatment plant were abandoned before the calibration and verification studies were completed. Consequently, no production runs of the model were conducted to assess discharge quality alternatives for the proposed plant.

Though the developed model was not used to achieve the original goal of the study, several important recommendations were made regarding future model use. These were:

1) External sources and sinks of nutrients should be better defined,
2) Additional phytoplankton sampling should be done to verify the model, and
3) Once these two steps are completed, the model should be applied to the Manasquan Estuary.

The problems in calibrating detrital-N and CBOD at Chapman's Wharf illustrated the need to better define external sources and sinks of nutrients. Potential sources and sinks would include non-point source discharges, sediment-water exchanges, and marsh-estuary exchanges. This last potential source/sink could have been significant in the upper portion of the estuary, where the estuary is shallow and the tidal portions include marshlands. The other major observation made by the modelers was that a more complete set of data would increase confidence in the model . With additional phytoplankton sampling, model simulation of the algal species could be verified, and the model's simulation of nighttime estuary activity could be evaluated with round-the-clock sampling data. Once the additional data were obtained, the recommendations were made that the model be used to:

(1) Determine the existing and potential impact of nonpoint source pollution within the Manasquan River Basin and

(2) Evaluate the potential impacts of proposed reservoir development within the basin on the downstream Manasquan Estuary.

12.4 References

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Thatcher, M.L. and Harleman, D.R.F. February 1972. "Mathematical Model for the Prediction of Unsteady Salinity Intrusion in Estuaries," Technical Report No. 144, R.M. Parsons Laboratory for Water Resources and Hydrodynamics, Department of Civil Engineering, M.I.T., Cambridge, MA.

Thatcher, M.L., and Harleman, D.R.F., February 1981. "Long-Term Salinity Calculation in Delaware Estuary," Journal of the Environment Engineering Division, ASCE, Volume 107, No. EE1, Proc. Paper 16011, pp. 11-27.

13. Calcasieu River Estuary Modeling

13.1. Background

The Calcasieu River Estuary modeling study is presented here to illustrate a time-variable waste load allocation model applied to a complex Gulf of Mexico estuary. The general model framework of RECEIV-II (Raytheon, 1974) was used to model simulate a forty-mile stretch of river from the salt water barrier near Lake Charles, Louisiana, extending downstream to the Intracoastal Waterway (shaded area in Figure 13-1). The primary water quality problems were the result of point source discharges. There were 64 wastewater dischargers to the Calcasieu River below the salt water barrier. In the forty-mile study area, there is a seven mile reach (between river miles 24 and 31) characterized by depressed dissolved oxygen concentrations, elevated temperatures and elevated ammonia concentrations. The water above the salt water barrier also suffers from low dissolved oxygen.

The poor water quality and the complexity of the system has led to a series of water quality modeling studies on the Calcasieu. Prior to the development of this model, four other water quality modeling studies had been completed on the Calcasieu. The first study was reported in January 1974 by Roy F. Weston, covering the entire Calacasieu River basin. It used a nomographic (graphical) technique for preliminary waste load allocation. A 1980 study was conducted by Hydroscience as part of a state-wide water quality planning effort. This second model was an improvement over the first, but it lacked a hydrodynamic module and relied on the modeler to specify flow conditions. Hydrodynamic data were very limited. In 1981, AWARE Inc. completed a third water quality model of the Calcasieu River estuary for the section below the salt water barrier using a two-dimensional application of the RECEIV-II model. The model was later used by Roy F. Weston for waste load allocation analysis. The focus of the study described herein is a more recent use of the RECEIV-II model for the Calcasieu River basin (Duke, 1985). Duke built on the work of AWARE and Weston by improving the calibration procedure and using new estuary cross-section information.

13.2. Problem Setting

13.2.1. Site Description

The Calcasieu River estuary is a complex system of natural and artificial channels. From its headwaters near Slagle, the Calcasieu River flows southward for 160 miles to the Gulf of Mexico. The study area for this model application was the lower 40 miles of river, below the salt water barrier (Figure 13-1).

The Army Corps of Engineers constructed the barrier and maintains a dredged ship channel to a depth of 40 feet and bottom width of 400 feet in most of the estuary. Stretches of the natural channel not dredged for the ship channel are referred to as "loops" or "lakes." The system is a tidal estuary with extensive side channel and reservoir-like storage. Side channel and tributary hydraulics are complicated by man-made channels and the main channel flow is complicated by the presence of large lakes.

High flows in the Calcasieu occur in the winter and low flows occur in the summer. There are no permanent stream flow measuring stations in the study area, although six tide gages measure water levels. A seven day, ten year drought flow (7Q10) was calculated using relative drainage area sizes and the drought flow of the nearest upstream gage station (Kinder, LA). The drainage area above the salt water barrier is 3,100 square miles. The nearest upsteam station has a long

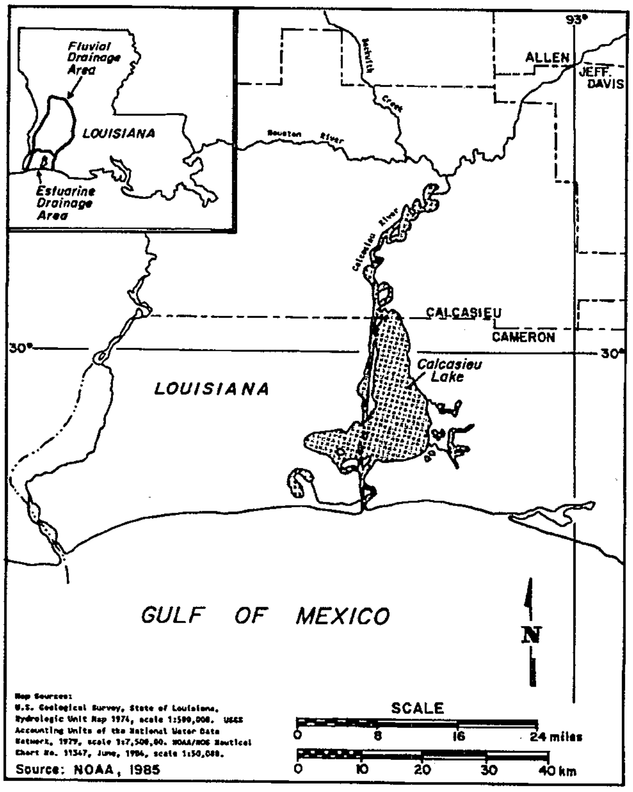

Figure 13-1. Calcasieu Estuary study area [NOAA (1985)].

term mean flow of 2,600 cfs and a 7Q10 of 202 cfs. The 7Q10 below the salt water barrier was estimated to be 375 cfs.

13.2.2. Water Quality Monitoring

The State of Louisiana conducted six water quality surveys at 31 stations during the following periods:

- July 1978
- October 1978
- July 1979
- August 1979
- July 1980
- June 1984

At each station, the following ten constituents were measured and simulated in the model:

1) Water temperature
2) Salinity
3) Dissolved Oxygen
4) BOD
5) Phosphorus
6) Nitrites
7) Nitrates
8) Ammonia
9) Total Kjeldahl Nitrogen
10) Chlorophyll *a*

Vertical profiles were measured for salinity, temperature, dissolved oxygen, pH, and conductivity. The June 1984 study was the most comprehensive. It was done in conjunction with six other studies that included a nonpoint source survey, a nitrogen transformation study, a sediment oxygen demand study, a use-attainability study, a series of mini-surveys for *in situ* water quality parameters, and additional hydrodynamic studies. All studies had municipal waste load data, although only the 1984 study included a full set of waste load data from all industrial discharges.

The water quality studies showed that the ship channel below the salt water barrier was stratified with respect to salinity and dissolved oxygen. The channel had once been thermally stratified, but this had been reduced because of the removal of cooling water discharges.

The estuary water quality was characteristic of water receiving wastewater effluent — high nitrite/nitrate, phosphorus, and BOD, and low dissolved oxygen. In the upper half of the estuary (below the saltwater barrier) dissolved oxygen was below the State's 4.0 mg/l standard. Phosphorus and nitrogen concentrations were characterisitic of eutrophic conditions. Phosphate ranged from 0.1 to 0.3 mg/l. Ammonia concentrations ranged from 0 to 0.6 mg/l. Much of the degraded water quality was from loading upstream of the saltwater barrier.

13.3. Model Application

13.3.1. Model Framework

The model selected for the Calcasieu was RECEIV-II. It is a time-variable model developed from the receiving water component of U.S. EPA's SWMM model. It was modified by Raytheon (1974) for use on 28 New England rivers and harbors. The 13 subroutines that form the model remain compatible with SWMM, but can be run independently. The model has the following general characteristics:

- Time variable water quality and hydraulics
- Eleven water quality variables (conservative and nonconservative)
- Link-node approach (vertically homogenous)
- Multiple tidal forcing points

The model has both a hydraulic and water quality component. For hydraulics, the model uses a link-node approach. Each node or junction is connected via links or channels. The equation written for each link incorporates fluid resistance and wind stress using the Manning and Ekman equations. Both components use a finite difference solution. The hydraulic component requires considerably more computer time than the water quality component because computations are performed for the entire system for time steps of five minutes or less, whereas the water quality component uses a one-hour time step.

For the Calcasieu, the RECEIV-II model framework was used without major changes from that documented by Raytheon. Certain changes to the FORTRAN source code were required to tailor the hydrodynamic module for site-specific characteristics.

13.3.2. Procedures

The model was calibrated with the data set from August 1979. It was verified using July 1978, July 1980, and June 1984 data sets. The model was recalibrated by revising the selection of model coefficients and extending the modeled area farther upstream at each tributary to improve the representative network of water storage in the system (Figure 13-2). The model has 67 load sources, 162 links, and 114 nodes. The number of cycles of the simulation were increased because the short simulations of earlier modelers had not achieved steady-state.

Model simulations were conducted at steady state for several reasons. First, insufficient data were available to calibrate or verify dynamic conditions. Second, model projections were to be run at 7Q10 steady state conditions. This assumption of steady state critical conditions is consistent with regulatory policy to use

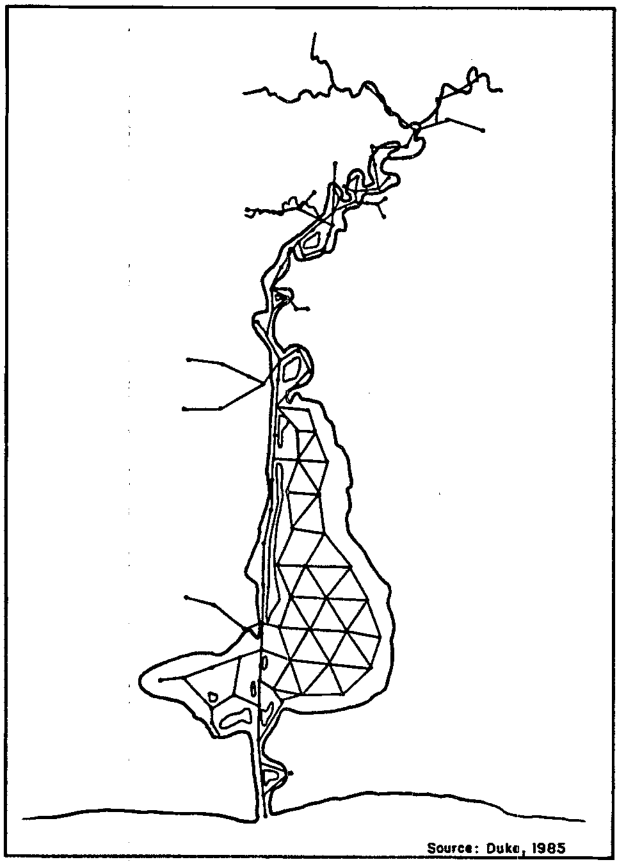

Figure 13-2. Model segmentation diagram [Duke (1985)].

conservative assumptions protective of the environment when dealing with model uncertainty.

Before proceeding with model calibration, the model was tested to determine if the thirteen day simulation used in earlier studies was a sufficient amount of time to achieve steady-state conditions. The initial salinity concentration was set to zero and a salinity wave was propagated upstream from the Gulf, downstream from the barrier, and from tributary inflows. After 13 days, salinity was still simulated near zero, indicating a 13 day cycle was not sufficient to achieve steady state. To ensure steady-state conditions, Duke ran the simulations for more than 900 days. This required approximately 4 hours of CPU time on the Louisiana DEP Digital VAX 11/780 computer.

Model rate coefficients were first adjusted to best simulate the August 1979 calibration data set. When model output matched observations within acceptable limits, model verification simulations were tested. In model verification, rate coefficients were identical to the calibration, but environmental conditions and loadings were adjusted to reflect the specific verification surveys. These changes included:

- Tributary flows and loads
- Upstream flows and loads
- Waste discharge flows and loads
- Ambient temperatures

The model was run for each verification survey and compared with the field data. Whenever a model parameter was changed during the verification, all data sets were run again to ensure the change did not significantly change the simulation of any data set.

The major coefficients are summarized in Table 13-1. These values were changed spatially within each survey but not changed from survey to survey. Model inputs for forcing conditions (e.g. tides, temperatures, flow, etc.) and loading were as measured for each survey.

13.3.3. Calibration/Verification

The results of the model calibration/verification are summarized in a few representative plots. The calibration/verification was described as good for hydrodynamics and fair for water quality. Obvious discrepancies between the data and model were seen for both selected hydrodynamics and water quality simulations, but not viewed as a serious problem. Problems with poorly defined loads was one complicating factor. In addition, model predictions were for steady state conditions, while observed data reflected dynamic conditions.

Comparison of the results from the calibration and verification simulations were divided into ship channel simulations and other stations. The other stations included the lake and loop areas. The results of the other simulations were not presented by the author since they were described as similar to the main ship channel. Also, tidal water quality calculations were performed but only tidally averaged results were compared to data.

Table 13-1. Values for Major Coefficients

Coefficient	Units	Range
Manning's n	none	0.018-0.035
Ammonia Oxidation	per day	0.002-0.020
Nitrite Oxidation	per day	1.00
BOD Oxidation	per day	0.001-0.050
Benthic Oxygen Demand	gm/sq.m/day	0.75-1.50
Reaeration	per day	0.003-2.000

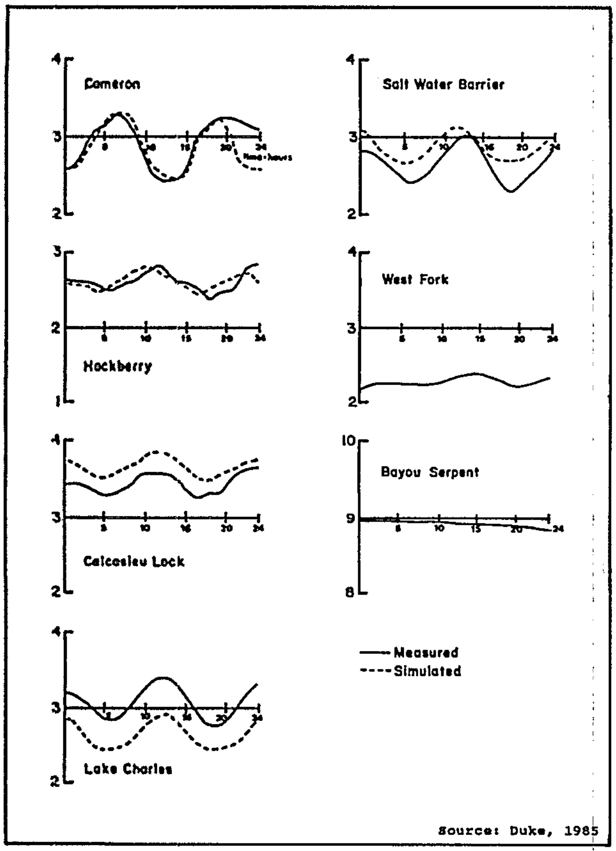

Figure 13-3. Tidal stage results for August 1979 hydrodynamic calibration simulation [Duke (1985)]

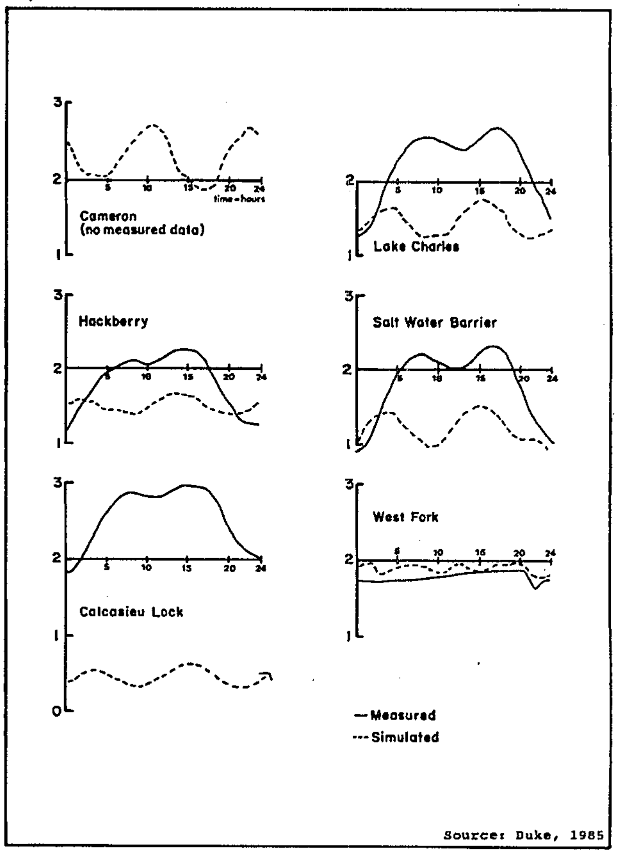

Figure 13-4. Tidal stage results for hydrodynamic verification simulation (July 1978 data set) [Duke (1985)].

Hydrodynamics:

The model calibration results for August 1979 hydrodynamics are summarized in Figure 13-3 for five stations below the salt water barrier. Model performance was measured using water elevations. The model was considered a satisfactory match to data since the trends and timing were well matched. The elevation differences were considered insignificant. The model verification comparisons were similar for July 1980 and June 1984 in that the model matched the trends well but was inconsistent in matching the magnitude. However, for the July 1978 data set (see Figure 13-4) the cycles and magnitudes were poorly matched. Overall, the hydrodynamic calibration/verification was described in the final report as good.

Water Quality:

The water quality calibration/verification simulated the ten parameters described above (Figures 13-5 through 13-9). Figures 13-5 and 13-6 are selected model comparisons for a few parameters from the August 1979 model calibration. Figures 13-7, 13-8, and 13-9 are selected results for the three verification simulations.

The water quality calibration/verification match was characterized as fair, with many discrepancies attributed to poor information on loading conditions and dynamics.

13.3.4. Model Sensitivity

An important modeling activity is sensitivity analysis. This procedure tests the sensitivity of model calculations to changes in selected inputs. Results can be used to:

- Refine coefficient selection
- Identify the most important processes and loads
- Identify areas in need of better data to improve modeling
- Define model uncertainty

The model was tested for an elimination and tripling of BOD and ammonia deoxygenation rates and elimination of algae. The results indicated that algae had the largest effect on the water quality calculations. This finding is common to estuaries where algal abundance often is the major factor in controlling water quality. As a result, success or failure in model validation to data

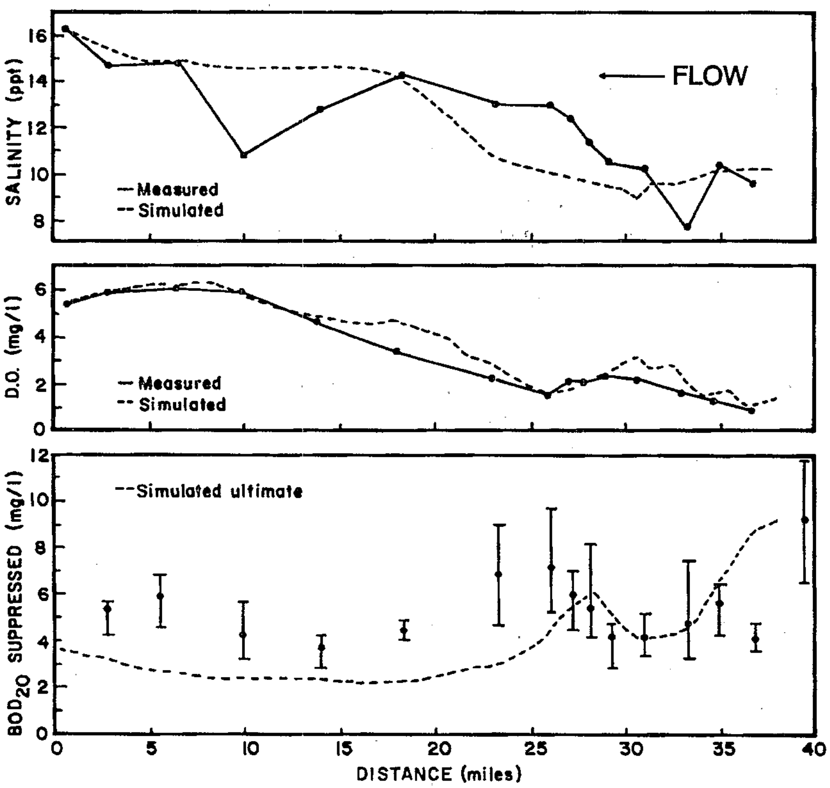

Figure 13-5. Selected water quality results for calibration simulation (August 1979 data set); salinity, dissolved oxygen, and biological oxygen demand [Duke (1985)].

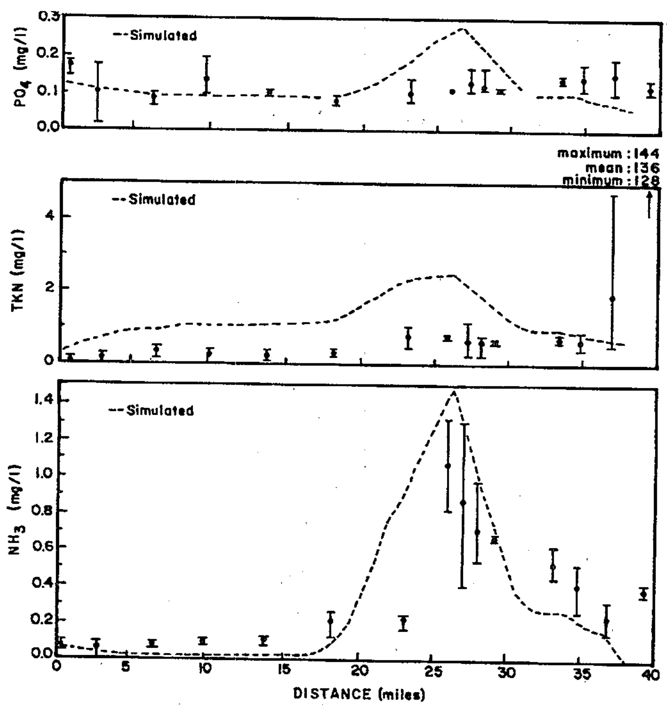

Figure 13-6. Selected water quality results for calibration simulation (August 1979 data set); phosphate, total Kjeldhal nitrogen, and ammonia [Duke (1985)].

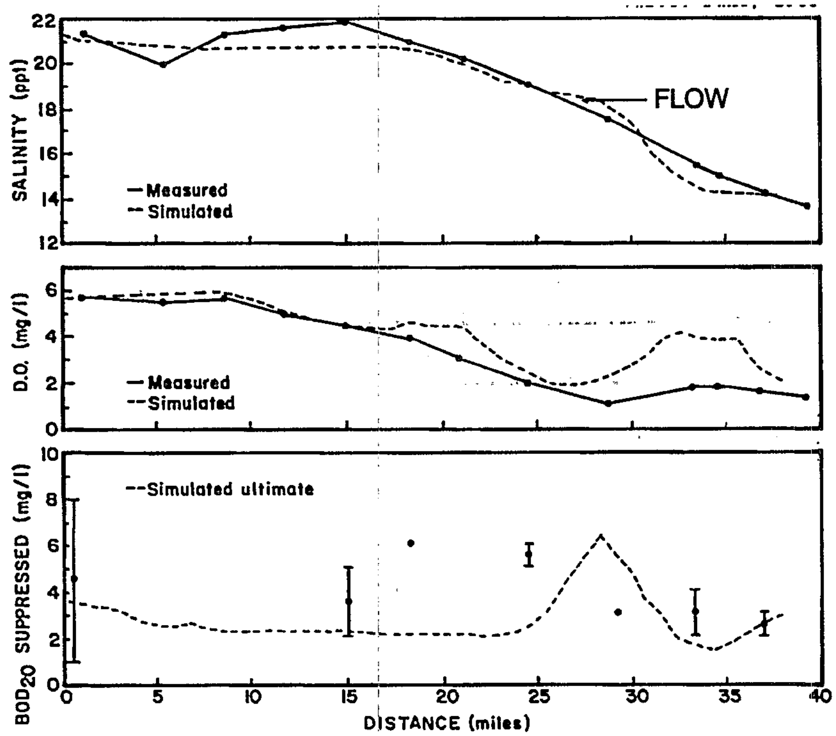

Figure 13-7. Selected water quality results for July 1978 verification simulation; salinity, dissolved oxygen, and biological oxygen demand [Duke (1985)].

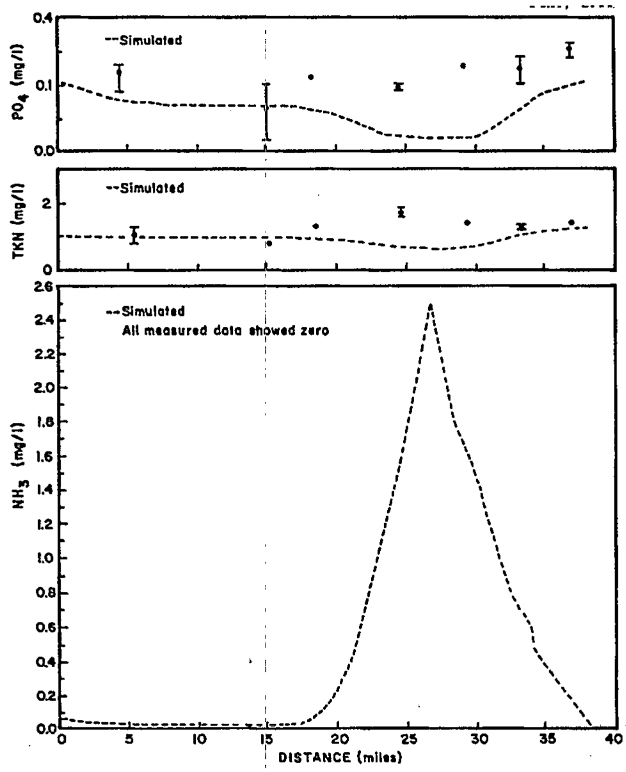

Figure 13-8. Selected water quality results for July 1978 verification simulation; phosphate, total Kjeldhal nitrogen, and ammonia [Duke (1985)].

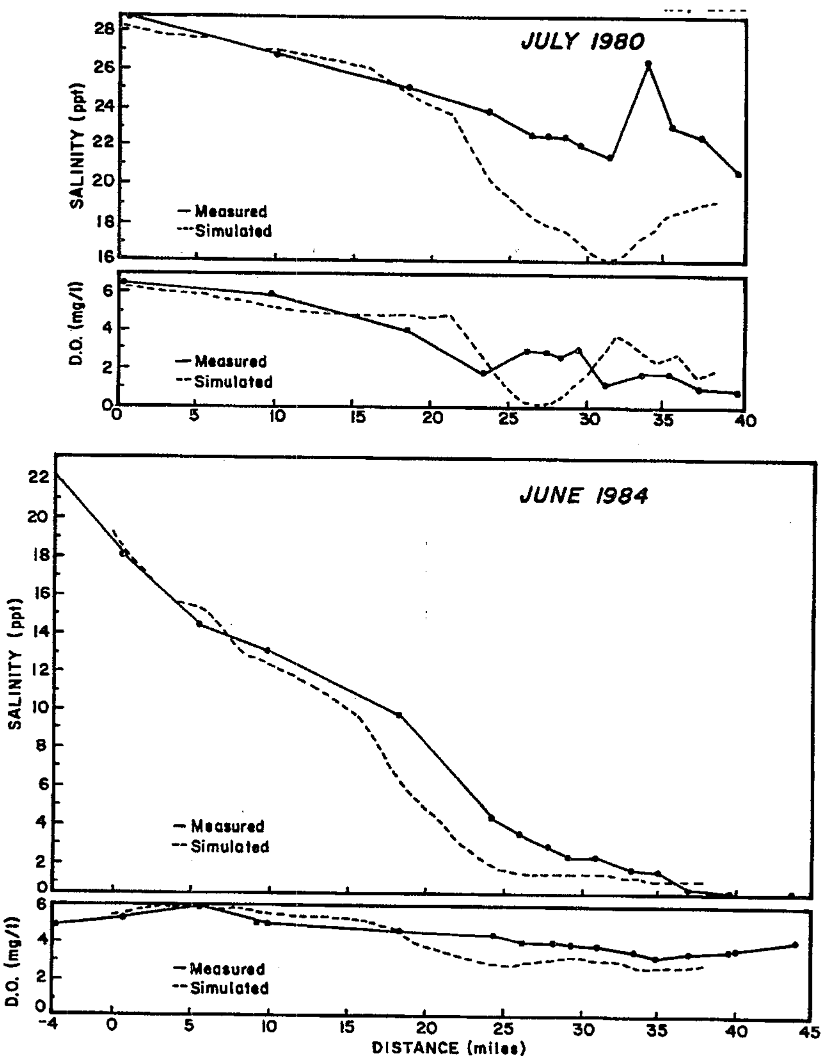

Figure 13-9. Selected water quality results for July 1980 and June 1984 verification simulation; salinity and dissolved oxygen [Duke (1985)].

can depend on proper characterization and simulation of algal dynamics.

13.4. Total Maximum Daily Loads

The purpose of all modeling efforts on the Calcasieu was to develop total maximum daily loads (TMDL) and wasteload allocations. In the earliest study by Weston (1974), the TMDL for the Calcasieu River was calculated to be 31,190 pounds ultimate oxygen demand per day (lbs UOD/day). Fourteen municipal and industrial dischargers were then allocated waste loads for BOD and NH_3-N.

In 1980, Hydroscience produced general recommendations on waste load allocation rather than determine specific TMDL. They emphasized the need to regulate the area with respect to dissolved oxygen. The study concluded that background loads were so high that even at zero discharge below the salt water barrier, a DO standard of 4 mg/l would not be met. Despite the lack of a TMDL from this modeling study, the 1980 Water Quality Management Plan for the State of Louisiana listed a TMDL for the Calcasieu River of 52,760 lbs UOD/day based on a dissolved oxygen standard of 4 mg/l. The second Weston study that followed the AWARE 1981 modeling agreed with the Hydroscience report, computing a zero TMDL because of a violation of the standard at zero discharge. A use attainability study (Thompson and Fitzhugh, 1986) demonstrated that waters above the salt water barrier are naturally dystrophic. The Duke study, in concurrence with the State and EPA, developed the TMDL to protect against the oxygen sag which occurs near river mile 26. Using the 4 mg/l DO standard and 1979 loading pattern, the Duke study produced an estimated TMDL of 83,130 lbs UOD/day.

13.5. References

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14. Expert Critique of Case Studies

Estuarine modeling is a complex and evolving science. As such, there is not total agreement among experts in the field regarding the "proper" approach to estuarine waste load allocation modeling. This chapter presents the **opinions** of three nationally recognized experts in estuarine modeling. These experts were asked to provide their thoughts on the proper approach to estuarine WLA modeling in general and to the case studies provided in this guidance manual in particular.It should be noted that the case study critiques are based primarily upon the studies as described in this document. They do not necessarily consider potentially important factors such as resources or time available to perform the modeling.

The reader is encouraged to examine these reviews and to compare and contrast the expert opinions. While all three experts are in agreement with the basic guidance provided in Parts 1 through 3 of this manual (each having served as a technical reviewer), their specific approach to estuarine WLA is seen to differ. Readers should therefore be aware that while this manual provides a general background to estuarine modeling, the exact approach to be taken for any given site still requires some subjective assumptions.

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14.1.1. Introduction

My overall opinion on the appropriate level of estuarine water quality model complexity can be summarized by the observation that:

THE BEST MODELS ARE OFTEN THE SIMPLEST

The review therefore will continually display a bias towards doing estuarine water quality modeling in as simple a fashion as possible and only after all simplicity has been exhausted, should increasing complexity be introduced and then only after careful consideration is given to the improvements in the model that might be realized. The reasons for this bias are: (a) most analysts have only limited experience, time and resources available, and (b) unnecessarily complex models sometimes tend to obscure uncertainty behind a facade of "reality."

The choice of the appropriate level of model complexity is determined in large measure by the nature of the problem under investigation. The context for my opinion on an appropriate level of model complexity is the establishment of a defensible analysis framework for a Waste Load Allocation (WLA). The opinion is not directed toward model development in a research context. This is not to say that one need not pay any attention at all to the scientific correctness of the model. Rather, modeling for WLA purposes imposes a separate, but related set of constraints on the model construction and development.

The assignment of a WLA to a particular discharger or regional group of dischargers involves a determination of the level of treatment over and above secondary treatment and/or Best Practical Treatment (BPT) and Best Available Treatment (BAT) coupled with a specification of the allowable mass loading and/or effluent concentration. Nonpoint and transient sources may also be a part of the WLA. The primary thrust of modeling then for WLA purposes is from a control engineering point of view. The modeling is not necessarily conducted for a detailed understanding of the various interactive processes that may be operative (e.g., the dynamic behavior of nitrifying bacteria), but rather an engineering-scientific approximation to the real estuary which will provide a firm basis for the WLA. Therein lies the difficulty.

The analyst must make a delicate determination between the degree of complexity necessary for a defensible WLA, the time frame and budget available for completion of the WLA and the natural urge to continue to explore various components of the problem. Because of the skill needed to make this determination and the limited resources that are usually available, I would generally lean in the direction of more simple models rather than more complex models.

A. The Difference Between a Site-Specific Model and a Generic Model

One of the more troublesome aspects of contemporary estuarine modeling is the confusion that exists between (1) a mathematical model of a particular estuary with its unique setting and (2) a generic non-site-specific model embodied in a computer code that incorporates the principal components of water quality theory but in a completely general way. For purposes of this opinion, a model is defined as the application of accepted principles of water quality fate, transport and transformation theory, together with appropriate determination of site-specific parameters to predict water quality under some future conditions for the given estuary. A generic model is considered to be a general programming framework which also incorporates the basic theoretical components, but has no utility in a WLA until applied to a specific problem setting. The computer code of a generic model is transportable, a model of a given estuary is not.

Thus, it does not make much sense to refer to models of Boston Harbor and Appalachicola Bay as "WASP 4" models. The WASP 4 computing framework may have been used in both cases, but any other suitable computer program (with similar fate and transport processes) could have been used as well. The structuring of a water quality model for Boston Harbor requires much more than a simple choice of computer code. This opinion on model complexity is not directed therefore to issues associated with how to choose an appropriate computer code. Instead, my opinion is focused on the issues associated with determining the level of complexity for modeling a specific estuary or coastal water body always in the context of a WLA.

B. Analytical and Numerical Models

There are fundamentally two types of water quality models: analytical models where the solutions to a differential equation or set of differential equations are available, and numerical models where approximations are made to the derivatives of the operative differential equations. Analytical models are available only for relatively restrictive conditions, usually one dimensional, constant parameters and steady state, although solutions for some time variable inputs exist, again for restrictive situations.

It is interesting to note that the accompanying case studies do not indicate any use of analytical solutions to determine initial expected responses or to check on numerical model results. I do know, however, that analytical solutions were used for Saginaw Bay as a completely mixed bay exchanging with Lake Huron and the results provided important initial guidance for further model development. Similarly, analytical solutions were often used in the Potomac case to check on numerical model output in the initial stages of model construction. One wonders whether some of the calibration difficulties of some of the case studies would not have been alleviated by initial analytical checks on the order of water quality response to "close in" on which particular phenomena were of importance in describing the observed data.

In spite of the severe assumptions that must be invoked, it is strongly suggested that:

ANALYTICAL SOLUTIONS SHOULD BE USED TO COMPUTE INITIAL RESPONSE AND TEST NUMERICAL MODEL COMPUTATIONS.

Such computations provide the first approximations to the order of water quality response that might be expected from input loading under different hydrological regimes and model parameters. Also, the use of analytical models provides a first order check on more complicated numerical models to determine whether the numerical computations are approximately correct.

C. Model Evolution

The use of models in decision making must recognize that, very often, the understanding of estuarine processes, and the availability of data and model frameworks for a given estuary are always changing. Models are not static, but rather continually evolving. Decision makers must be apprised of this fact and must, to some degree, be prepared for new input into the decision process.

The Saginaw Bay and Potomac estuary case studies are good examples of models that began at relatively simple levels of complexity and have subsequently progressed to more complex kinetics and spatial and temporal detail. The progression was dictated by an ever increasing level of complexity in the questions being asked of the model. For example, the early Potomac estuary models did not explicitly include phytoplankton dynamics. But after issues of nutrient controls (e.g. should phosphorus or nitrogen be removed?) were raised, an expansion of existing models was required. However, as noted below, it is not always clear that adding additional complexity improves credibility. Thus, for the Saginaw Bay model, it is not clear that the addition of an internal nutrient pool state variable improved the model performance, whereas the inclusion of phytoplankton functional groups was important in predicting the occurrence of nuisance odors.

The Calcasieu estuary case study, on the other hand, seems to be an example of a modeling framework that needs to be substantially restructured (e.g. inclusion of a vertical dimension and non-steady state) in order to provide more credible results. Yet the original model (albeit with some updates) continued to be used with results that were less than desirable.

It should then be clearly recognized by all concerned (decision makers, model analysts and scientists and engineers) that:

ALL MODELS MUST CONTINUALLY BE UPDATED: IF NOT, MODEL "ATROPHY" SETS IN AND CREDIBILITY DETERIORATES. ESTIMATED MODEL "HALF-LIFE" IS ABOUT 1-2 YEARS.

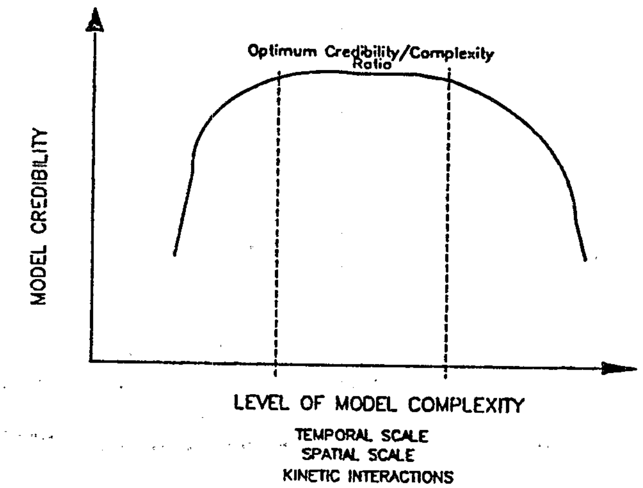

Figure 14-1. Illustration of relationship between model credibility and model complexity.

Existing models must therefore never be "frozen" in time and continue to be used in the face of obvious model inadequacies. As painful as it may be, some model frameworks need to be restructured, expanded or even abandoned as new information becomes available.

14.1.2. Appropriate Spatial and Temporal Scales

Unfortunately, because of the ready availability of computer programs that are fully time variable and three dimensional, there is a tendency to believe that more complexity is better since it approaches the real world more closely. But, increasing complexity does not usually result in increased model credibility. Figure 14-1 illustrates this opinion. In general, increasing model complexity requires specification of more and more parameters and state variables, both in absolute number and over space and time. Even more importantly, increased model complexity requires a detailed data base across all state variables and over space and time for a complete assessment of model adequacy. As a result, what appears to be more realistic is actually a model that has hidden within it a large degree of uncertainty. Because of a generally sparse data base, the uncertainty is not visible and it is assumed that the model is more realistic when in fact it is not.

On the other hand, the model may be so crude in spatial, temporal or kinetic definition that key mechanisms or issues associated with the problem are completely missed. Thus, a representation of a longitudinal estuary as a single completely mixed body of water is quite inappropriate since the impact of a load over distance is lost. Similarly, a steady state approximation may be completely incorrect because of the dynamic nature of the problem (e.g. time variable phytoplankton behavior).

The "art" of water quality modeling in general, is to carefully evaluate the relevant scales of the problem. This evaluation requires an assessment of the requisite degree of complexity as opposed to merely assuming that fully time variable, fine space scale models with extensive kinetic detail are always the best choice.

A. Temporal Scale Issues

Estuaries exhibit a variety of time scales: hour to hour, tidal and diurnal fluctuations, week to week and seasonal variations and year to year differences. From a modeling point of view, what are the choices? One can try to represent the entire time spectrum from short term to long term behavior, but this is clearly impractical. A model may concentrate on the short term, intratidal and diurnal variations, with a possible loss of focus on the longer term phenomena. Conversely, a steady state model may miss the transient effects of storm water inputs or transient hydrologic events. The choice of relevant model temporal scale in my opinion centers about the use of estuarine modeling for WLA purposes.

A WLA may be a constant (over time) effluent concentration or a seasonal variation may be allowed (as in seasonal nitrification). These specifications are usually assigned to meet water quality objectives during some critical flow and temperature period. It is not usual to assign a WLA on a short time scale with the exception of a probabilisitic assignment of maximum values not be exceeded. Also, WLA analyses often need to be conducted with relatively limited data, which are usually not of sufficient density in time and space to calibrate a fully time variable intra-tidal model. Rather, data are more frequently available at irregular time intervals, but with some spatial definition. Finally, developing fully time variable models at an intra-tidal level is a complex time consuming effort with a necessity to conduct extensive data analysis and output processing in order to display model results in a defensible manner.

The case studies show a range of temporal scales, from the steady state analyses of the Calcasieu estuary to the intra-tidal models of the Manasquan estuary and DO and total residual chlorine in the Potomac estuary.

The intra-tidal choice for the Manasquan (over two 4-day periods) is not considered to be the correct choice since the water quality problem under study involved kinetic behavior over time scales of weeks and seasons. Key behavior is therefore not captured by the temporal scale of the Manasquan model. Also, the fact that intra-tidal computations were performed does not, in itself, provide for an accurate representation of the actual variability in the data. Indeed, it is not clear from the comparisons to data presented in the case study that the intra-tidal calculations captured the actual variability with any substantive degree of success.

The choice of an intra-tidal scale for the total residual chlorine in the Potomac is correct since the kinetics of the disappearance of chlorine are quite rapid. The time variable behavior of the chlorine state variable thus needs to be calculated over short time intervals in order to model the expected transient behavior.

B. Spatial Scale Issues

The choice of spatial dimensionality and scale involves evaluation of available data (to determine significant gradients) and the expected geographical extent of the problem. The fineness of the spatial extent of the model is to some degree coupled to the temporal issues noted above. Generally, long time scale problems may involve larger scales and less detailed spatial definition.

The chlorine model of the Potomac is an example of where cross-estuary gradients needed to be computed necessitating a spatially detailed model in the lateral and longitudinal direction. The Saginaw Bay model consisting of five segments is a good example of a reasonable grid since a finer spatial definition would probably not contribute to any improved model credibility.

Finally, a remark should be made about model boundaries. The extent of the model should always be sufficiently far removed from any existing or proposed inputs that may be subject to a WLA. The boundaries should be at a point where the flows and exchanges and state variable concentrations can be specified and are independent of the model output. For example, it is not entirely clear from the Manasquan case study that the model boundary is proper, i.e. the extent of the model may have to be extended out past the inlet in order to provide a proper independent boundary condition. This may be especially true if the model had ever been used for analysis of the proposed regional input at the head of tide.

C. Suggested Strategy for Temporal-Spatial Scales

Since the principal reason for estuary modeling in the context of this opinion is a WLA, the following strategy for choosing a relevant temporal-spatial modeling scale is offered.

**TEMPORAL-SPATIAL SCALES
BEGIN WITH STEADY STATE,
"LARGE" SPACE SCALES,
THEN SEASONAL,
MORE DETAILED SPATIAL DEFINITION,
THEN INTRA-TIDAL, FINE SCALE.**

It is suggested that the temporal scale of most WLA estuarine models should begin at steady state to determine overall relationships between input loads and resulting water quality. Steady state is suggested even for highly reactive variables since the steady state modeling helps to define overall response levels and spatial extent of the input loadings.

Following steady state analyses, if time variable analyses need to be done in estuaries (as a result, e.g. of a need to specify phytoplankton dynamics for nutrient control or a seasonal WLA) then a seasonal time scale (with a model framework representing an average over a tidal cycle) should be used.

Only if the justification is quite clear, (e.g., transient storm water input analyses or a complicated hydrodynamic regime as in the Potomac estuary chlorine model) should an intra-tidal model be constructed. The fact that the estuary has a tidal oscillation is in itself not justification for constructing an intra-tidal model. The reason is threefold: (a) as noted earlier, the focus here is on WLA problems which are normally limited in resources, time and money, (b) most WLA problems involve processes that have longer time scales than tidal, and (c), there are many other sources of temporal variability in water quality that are not captured by intra-tidal calculations (e.g. hour to hour and highly local changes in solar radiation, suspended solids, wind, or velocity, among others).

It is suggested that initially a relatively crude spatial representation (e.g. a numerical grid size of several miles) be used for estuaries in the longitudinal direction in order to provide a rapid understanding of the expected order of water quality variations. If vertical gradients are significant, the model should include a vertical dimension at the outset. Only if warranted by the problem context should a spatially detailed (e.g. on the order of hundreds of feet) model be constructed.

14.1.3. Need for Hydrodynamic Models

Several of the case studies (e.g., Potomac, Manasquan and Calcasieu) make use of hydrodynamic models. Indeed, the case study reviews seem to imply rather consistently that a water quality model is always better when a hydrodynamic model is included. I do not agree that this is always true. It seems that a mathematical model of the hydrodynamics of the estuarine system is necessary when:

(a) the transport regime is complex in space and time and cannot be easily specified a priori,

(b) the transport regime will be changed under some future WLA condition, such as occasioned by channel deepening or straightening, or construction of barriers

(c) the absence of hydrodynamic model would weaken water quality model credibility in the eyes of a peer scientific review.

It is not clear that hydrodynamic modeling was crucial and essential for the Potomac DO and the Manasquan models. Indeed, the issues of water quality model credibility for a WLA often have little to do with the hydrodynamic calculation. Rather model credibility centers around (a) issues of water quality model calibration that do not depend on hydrodynamics (e.g. parameter specification), (b) inclusion of correct mechanisms (e.g. appropriate state variable or sediment source/sink interactions) and (c) point and nonpoint input load estimates. An alternate to a full hydrodynamic model calculation on an intra-tidal basis is to calculate the net transport from the fresh water flow and estimate tidal dispersion coefficients by using salinity (or dye) as a tracer. Many estuarine WLA models have been successfully constructed using this type of average across tide approach.

14.1.4. Appropriate Level of Kinetic Complexity

In addition to temporal and spatial issues, one must also consider the need to include various levels of kinetic complexity in the model. Specifically a choice must be made of the relevant state variables to be included in the model and the nature of the interaction between the state variables. For example, for a DO model, should phytoplankton be explicitly modeled or input? For a phytoplankton model, should various functional groups be modeled or should total chlorophyll be used? Should sediment nutrient fluxes be calculated or input?

As a general rule, I would advise to:

**KEEP STATE VARIABLES TO A MINIMUM;
MODEL ONLY THOSE FOR
WHICH DATA EXISTS;
BUT ALWAYS INCLUDE THOSE STATE
VARIABLES WHICH WILL BE
IMPACTED BY A WLA.**

The case studies seem to have implicitly recognized this general rule, although there are some exceptions. The Manasquan model is clearly over-specified with state variables and kinetic interactions for the nature of the problem under study and the available data sets. The inability to calibrate to the phytoplankton state variables severely limits the utility of the model.

On the other hand, the initial Potomac estuary DO model did not explicitly include organic nitrogen, nor ammonia uptake by phytoplankton. Also photosynthetic DO sources and sinks were externally inputted, but these inputs were to be extensively impacted by a WLA for nutrients. The model could not therefore respond to the WLA questions associated with the affect of nutrient control on DO.

Sometimes a state variable must be included even if data are not available. For example, for a toxic chemical model, both dissolved and particulate chemical must be modeled. But data may not be available for the dissolved component because of concentrations below a detection limit. Nevertheless, both components need to be included in the modeling framework.

14.1.5. Calibration and Verification Issues

Of course, all of the above only has relevance when the model is considered to be "representative" of the actual estuary. Thus, the question of the calibration and verification of the model must be addressed. This is an area about which much has been written and discussed for several decades, all centered about the issue of whether a model has adequately reproduced the observed data.

A. When Is A Model "Calibrated" And "Verified?"

In my opinion, a model is considered representative of the real estuary when the key model state variables reproduce the observed data over a range of expected conditions and within expected statistical variability. Of course, this definition may not help at all. For example, what is the "expected statistical variability?" Perhaps the only answer is that model "unrepresentativeness" is obvious. We know when a model is **not** repre-

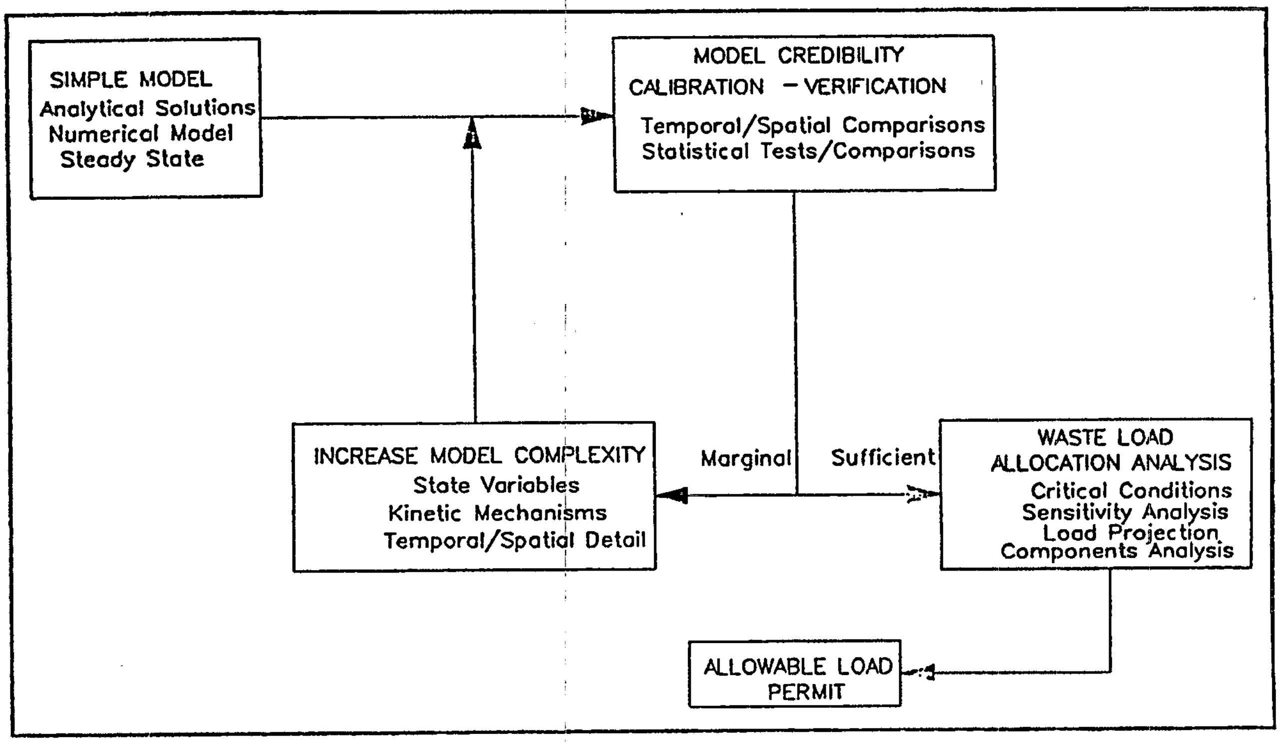

Figure 14-2. Suggested strategy for determining appropriate level of model complexity.

sentative. The Calcasieu case study is offered as an example of a model that is claimed by the analyst to be "good" for the hydrodynamic model and "fair" for the water quality model. But even a casual examination of the model comparisons to data indicate severe problems. The DO profile is not captured and a sag is calculated where it does not exist. This, in my opinion, is "unrepresentative" and outside the bounds of statistical variability.

Similarly, the Manasquan model simply fails in several state variables to bound the data. Also, the spatial profiles for this case are not presented so one cannot judge the adequacy of the model in reproducing longitudinal variability.

The Potomac estuary DO model was compared to various data sets by readjusting the model parameters for each calibration. This is unacceptable. The purpose of model calibration and verification is not to "force fit" the model to the data. Rather, the model parameter numerical assignment should obey the

PRINCIPLE OF PARSIMONY:
BE "STINGY" WITH THE SPATIAL AND TEMPORAL SPECIFICATION OF MODEL PARAMETERS AND HAVE A REASON FOR ALL ASSIGNMENTS.

The Potomac estuary phytoplankton and Saginaw Bay models offer extensive calibration and verification analyses, including various statistical measures of comparisons. Both spatial and temporal comparisons and statistics of comparisons are given. These case studies provide some measure then of an adequate representation of the data by the model and can be profitably used as a "model" of a model calibration. Two caveats are in order, however: (1) extensive data sets and resources were available in both cases, and (2) even with the extensive calibration and verification of the Potomac eutrophication model, a bloom in 1983 was not captured because of presumed pH mediated sediment phosphorus release, a mechanism not previously included in the model.

14.1.6. Summary

Figure 14-2 summarizes all of the above comments.

As indicated, the suggested procedure is to begin with simple representations of the estuarine system. This should always include some investigation of the estuary water quality problem with analytical solutions. This is true for all problem contexts. For DO, simple steady state solutions should be used to provide estimates of the impact on carbonaceous and nitrogenous loads, sediment oxygen demand, and photosynthesis and respiration on the DO. For nutrient problems, total nutrient calculations should be performed to determine importance of sediment fluxes and net loss from the water column. For toxics problems, total, particulate and dissolved chemical can be easily estimated.

If the estuarine system is too complex for initial analytical solutions (e.g. when vertical and lateral gradients must be defined) then a steady state numerical model is recommended. The spatial definition is determined from the gradients that need to be captured.

Following the structuring of the simple model, initial determinations should be made of the model credibility. Comparisons to data should be presented over the spatial dimensions of the model. Where appropriate, statistical measure of model adequacy should be computed.

The degree of model credibility should then be assessed in the light of the WLA.

THE SIMPLE MODEL MAY TURN OUT TO BE ENTIRELY SUFFICIENT FOR WLA PURPOSES.

If a determination is made that the simple model provides only "marginal" model credibility, then model complexity should be increased. This increase in model complexity often needs to proceed in the following order: (a) additional state variables, (b) additional kinetic interactions, (c) increased temporal and spatial definition. It is in the latter that hydrodynamic modeling may be necessary.

Additional calibration and verification is then conducted with the hope that model credibility is increased. This step should include, whenever possible, comparisons to data sets collected over a range of environmental and input loading conditions.

After a determination has been made, then a full WLA analysis can be conducted. This analysis should include evaluation of water quality response under critical design conditions, sensitivity analysis, projection of expected loads in the future and components analysis of individual inputs. This latter analysis is aimed at describing the relative contribution to the calculated response from individual components, e.g. particular point source inputs, and distributed sources (such as sediment sources). The analysis often provides key insights into which inputs and mechanisms are most important in the WLA. (None of the case studies displayed any components analysis).

The final outcome is then the recommended WLA for an input or region with associated permit specifications. It is this final outcome that should always be kept in perspective when assessing the need for various levels of model complexity. Ultimately, of course, the measure of success of the model is the degree to which the model projections are actually realized after the WLA has been implemented. But that is a topic for another opinion at a different time.

14.1.7. Case Study Review

Case Study 1 - Saginaw Bay

This case study is a very good example of a proper mix of spatial and temporal specification together with proper representation of kinetic detail. Illustrations of the extensive calibration of the model are given and the post audit of the model is unique. The statistical comparison between model output and data as shown in Table 10-4 is a very good example of what should be expected from a water quality model.

The use of a five segment model is entirely appropriate since the proper exchanges and transport were determined from measured salt concentrations. In this reviewer's opinion, a representation of the system with a finer grid operating at finer time and space scales would not improve the model performance and indeed may have considerably delayed and obscured the interpretation of model output.

It is concluded that the overall analysis of Saginaw Bay eutrophication as given in this case study is a paradigm analysis for water quality modeling. The modeling provided considerable insight into the dynamic behavior of phytoplankton functional groups, incorporated a detailed calibration and verification analysis and uniquely conducted a post-audit analysis after nutrient controls were implemented.

Case Study 2 - Potomac Estuary

This case study, a summary of three efforts on the Potomac estuary, illustrates a range of modeling approaches to estuarine water quality.

<u>DYNAMIC ESTUARY MODEL</u>

The first effort, the use of the Dynamic Estuary Model (DEM) examined the DO resources of the estuary. The one dimensional hydrodynamic model was used to provide the transport and was calibrated to hydraulic properties as well as the longitudinal extent of chloride concentration in the estuary. This effort is a good example of calibration of the model to observed data, but also indicates the hazards of calibration where the underlying kinetic structure is too simple. The DO calibration reset initial conditions for each survey. This is not considered a proper calibration method. As inidicated during a post-audit, the DEM failed to properly account for nitrification phenomena by assuming that all ammonia that was lost was due to nitrification, rather than through some measure of uptake by the phytoplankton. The intratidal hydrodynamic model, while initially appearing to provide a more realistic "real time" modeling framework, in actuality added little to understanding of the overall water quality behavior of the estuary.

The history of the DEM is a useful example of model evolution in the midst of decision making. With initial emphasis on intra-tidal calculations to a shift towards more detailed kinetic evaluations during the post audit stage, the DEM illustrates the need to properly include necessary phenomena that link various water quality constituents.

POTOMAC EUTROPHICATION MODEL

The Potomac Eutrophication Model (PEM) is an example of an intermediate scale of estuarine water quality model. The use of a coarse grid in the lower estuary was justified on the basis of the lack of any significant gradients in water quality constituents of interest. Vertical homogeneity is a key assumption and undoubtedly influenced the ability of the model to properly calculate water quality in the region of the turbidity maximum. This time variable model (on a time scale of weeks to seasons) properly did not rely on a detailed intra-tidal hydrodynamic calculation on a fine time and space scale. Emphasis was rather placed on the role of the sediment on the overlying nutrient concentrations and the interactions of the various nutrient forms with phytoplankton and DO.

The PEM study is a good example of extensive calibration and verification analyses, illustrations of which are shown in the case summary. Also, the PEM analysis made use of extensive statistical comparisons (see 11.4.6) between the model output and the observed data.

Like the DEM, the PEM was subjected to a post audit analysis. The analysis was prompted by a major algal bloom in the summer of 1983. As noted in the case study summary, pg. 11-12 ff., the PEM was not able to predict the full extent of the observed bloom, due in some measure to a significant source of phosphorus that was not incorporated in PEM. Subsequent work indicated that such a source may have been from a pH mediated release of sediment phosphorus. Additional input may have resulted from upstream transport of phosphorus from downstream bottom waters. This latter effect was also not included in PEM because of the vertically homogeneous nature of the model.

Overall, the PEM is a good example of calibration and verification of a time variable eutrophication estuarine system. It also illustrates the hazards of apparently "best" calibration of the model that misses a phenomena which only appears after certain conditions ensue. Nevertheless, the PEM proved useful in a variety of decision making contexts, not the least of which was to assess the reasons for the major 1983 algal bloom.

FINITE ELEMENT CHLORINE MODEL

This model is a very good example of the proper choice of time and space scales. Because the decay rate of chlorine is so rapid, the zone of influence of the chlorine residual would be expected to be highly local. As a result, this model has as its spatial focus a region of about five miles centered at the location of the major input. Detailed lateral specification is required because of the need to calculate lateral movement of the chlorine. Model calibration of transport and dispersion was first accomplished by comparisons to dye study results. The results shown in Figure 11-14 are a good example of what one can expect. The general shape is captured, but not all of the details even though the grid is relatively fine. As noted in the text, further work using dye decay would be necessary to improve the calibration. It was concluded however, that the dispersion was properly captured in general.

That conclusion is a good example of a judgement made by the analysts on the suitability of a model calculation. This reviewer believes that the judgement made here is correct, but only because of the calibration analysis to the observed dye data.

A similar conclusion can be drawn with respect to the calibration of the total residual chlorine model to survey data. What was required here was approximate representation of the general field of the chlorine, to approximate order of magnitude. This was achieved. More importantly, the sensitivity analysis indicated the degree of model uncertainty and this is clearly discussed. That uncertainty did not affect the basic conclusions.

SUMMARY

These three modeling efforts of the Potomac estuary water quality illustrate a good range of spatial and temporal scales, level of model complexity and the need for extensive calibration and verification to observed data. Two major points seem to emerge:

- Uncertainty in the model coefficients sometimes does not affect the conclusions, i.e., the decisions that are reached. But under certain situations, a model that is believed to be properly calibrated can miss entire phenomena or linkages. Such a model may then fail in varying degrees during a post audit. The experience of the Potomac esturary models summarized in this case study should be borne in mind by any analyst.

- Each problem requires its own spatial, temporal and kinetic level of detail. Finer spatial and temporal resolution is often not the issue especially when the problem context is over a larger time and space scale. Funding and project completion times are realities that must be faced in any modeling effort. Such constraints must be balanced against more and more detail in the modeling framework with perhaps less than desired return in improving the certainty of decision making.

Case Study 3 - Manasquan Estuary

This model illustrates the use of an intra-tidal calculation to describe estuarine water quality. This reviewer believes that the proper temporal scale was not used. By focusing in on two 4 day periods as examples of "calibration" and "verification," the model does not capture the longer term, i.e., week to month, behavior of the water quality constituents of interest. Further, the analysis is flawed in several ways. The August 1980 period is used as a calibration set and July 1980 is used as a verification data set. What would be much more convincing is to use the model in one complete calculation extending from prior to July 1980 through the August 1980 data. By restarting the calculation each time before August and July and then extending the calculation for only four days, the credibility of the model is severely compromised.

Also, this model is presented as a demonstration of a "successful calibration and verification of a real-time estuary model." This reviewer does not agree that this model is successfully calibrated and verified even for a brief period of four days. The "real time" model is presented in a fashion that seems to indicate that because the model calculated at a time scale of hours or less that it is more realistic than averaged models. Ostensibly, the "real time model was selected to predict photosynthesis effects on diurnal DO." But the model fails to reproduce the observed DO range (see e.g., Figure 12-9 and 12-10). Also, the CBOD, NBOD and nitrogen forms are not calibrated. For example, Figure 12-18 shows comparisons of computed nitrogen forms to observed data. The computed forms vary approximately sinusoidally with an apparent look of reality and certainty. But the comparison to the observed ammonium data, for example, show some significant over-calculation of the data. One wonders how well the model would have done if the model were not restarted for the July 1980 data set but rather was run for a several month period.

It is recognized that this model was apparently constructed with only limited data and under apparently tight constraints. As such, the exercise is useful in showing how a model can be used to delineate data and input load deficiencies. However, the modeling framework is not considered to be adequately calibrated and verified over the time scales necessary for the water quality constituents under investigation. The model spatial extent may also be inadequate for evaluating certain alternatives and may have to be extended into the ocean.

Case Study 4 - Calcasieu River Estuary

This case study is adequately presented as an example of a modeling context with problems in credibility and in application. The modeling structure is flawed in not adequately representing phytoplankton interactions on the DO, no settling of particulate forms and a lack of vertical detail. (No data are presented however to indicate the extent of any vertical stratification in salinity or DO). The model is not considered to be adequately calibrated and verified because of a failure to capture the salinity and DO profiles on several occasions. More critically, the conclusion on a total maximum daily load of 83,130 lbs UOD/day is not justified by the model analysis. Since the data already indicate DO violations below a standard of 4 mg/L, it is hard to see how the stated allowable load was determined.

This case study should be seen as an example of model evolution under different analysts with final results that are marginal at best. The difficulty stems from differences in the opinions of analysts as to what constitutes a satisfactorily calibrated and verified model. One analyst described the hydrodynamic calibration and verification as good, but this reviewer sees a very poor comparison. At several of the stations, the computed stage differs from the observed stage by several feet, an apparent clear inability of the model to properly represent the easiest of hydrodynamic variables. The adequacy of the hydrodynamic model can also be judged by examination of the salinity profiles which are erratic in comparison to observed data. For example, the July 1978 salinity profile is adequately captured, but the computed July 1980 profile is significantly below the observed data. A zero DO concentration is calculated in this vicinity that is not representative of the observed data.

In general, this case study indicates a modeling framework that is not entirely credible and as such, the application to a waste load allocation is somewhat problematical. The inconsistency of the computed allowable UOD load with the observed data, as noted above, is illustrative of the tenuous nature of the model for use in decision making.

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14.2.1. Introduction

The concept of a technical manual for performing wasteload allocation in estuaries is an excellent one. Part 4 of the manual is intended to be a "critical review of estuarine wasteload allocation modeling." It consists of four case studies "representing various levels of complexity." The task assigned to the reviewer is to provide a general discussion of the "appropriate level of estuarine model complexity" and to comment on the case studies within the context of the reviewer's philosophy of environmental modeling.

14.2.2. Statement of the Problem

Many environmental problems require the development of models in order to answer management questions related to the effectiveness of various control scenarios. Such an effort requires a careful statement of the problem and applicable regulatory constraints. Decision makers need to be able to assess the importance of controlling point or non-point sources of pollutants, and they usually need to know the time scale at which the estuary can be expected to respond to the implementation of source controls. Effective environmental modeling would avoid the Lake Mead fiasco where the City of Las Vegas operates a tertiary waste treatment plant designed to minimize phosphorus discharges to Lake Mead while the Fish and Wildlife Service periodically adds phosphorus to the lake to promote the growth of fish.

14.2.3. Data

Available data, both hydrodynamic and water quality, must be studied in order to understand the spatial complexity of the problem. In the hydrodynamic area, it is important to understand the factors influencing the currents and circulation pattern. These include: the degree of **vertical** stratification within the salinity intrusion zone, the extent of changes in **longitudinal** salinity intrusion due to tides, wind and seasonal changes in fresh water inflows, and the degree of **lateral** stratification due to fresh water inputs from tributaries located on one side of the estuary. Temperature stratification may also influence the vertical mixing and circulation pattern. The main stem of Chesapeake Bay is an excellent example of an estuary with distinctly three-dimensional characteristics.

In the water quality area, vertical stratification significantly affects the vertical flux of nutrients to and from the bottom sediments and may contribute to the formation of anoxic regions along the bottom of the estuary. The objective of the data analysis is a decision on the dimensionality of the model. It would obviously be inappropriate to use a two-dimensional depth averaged model in an estuary having a history of bottom anoxia.

14.2.4. Spatial Resolution of Models

In terms of spatial resolution, environmental models may be classified as box models or as one-, two-, or three-dimensional hydrodynamic models. The distinction between box models and the hierarchy of dimensional hydrodynamic models is an important one that is not clear in the presentation of the four case studies of Part 4.

A. Box Models

Box models require an empirical, rather than an analytical (or numerical), specification of the flow field. Thus there is no hydrodynamic model component in a box type model. Box models may be arranged in a longitudinal, lineal array or boxes may be arranged in pseudo two-dimensional depth-averaged arrays. Two examples of this are contained in the case studies. Case study 10.0 of Saginaw Bay on Lake Huron shows the entire Bay represented by five boxes (see Fig. 10.2). Case study 11.4, Potomac Eutrophication Model (PEM), uses a box network consisting of 23 main channel longitudinal segments and 15 lateral tidal embayment segments. In the lower saline portions of the estuary, these box segments are as much as 15 miles in length. This is mind-boggling when it is realized that, by definition, each box is a fully-mixed compartment.

Case study 10.0 (Saginaw Bay, Lake Huron) contains no information on how the flow between boxes (the largest of which has as surface area of about 400 square miles) or how the dispersive mixing parameters are determined. In addition, there is no information on the sensitivity of model results to these important transport quantities. The time scale of the model is seasonal, that is, it deals with monthly variations in water quality parameters. In terms of spatial and temporal resolution, it is difficult to see how this model would be applicable to estuary studies.

Case study 11.4 (Potomac Eutrophication Model) is similar to the Saginaw Bay study in that there is no information on how the daily averaged flow and dispersion between boxes is obtained.

In this reviewer's opinion, box models represent a "black art." Specification of empirical advective and dispersive transport between boxes can only be accomplished reliably by using a conservative substance such as salinity. Determining the spatial distribution of advection and dispersion for each box segment that satisfies a given salinity distribution requires the solution of an inverse problem for which there is no unique solution. Furthermore, the spatial distribution of advection and dispersion coefficients will change in time in relation to factors such as fresh water inflow, which change the longitudinal and vertical distribution of salinity.

B. Hydrodynamic models

The state-of-the-art of numerical hydrodynamic modeling is extremely well advanced in two-dimensional, both laterally averaged and depth averaged, applications. Limited, but reasonably good experience exists at the three-dimensional level. An excellent review of the status of two- and three-dimensional hydrodynamic modeling has been prepared by the ASCE Task Committee on Turbulence Models in Hydraulic Computation (ASCE, 1988). The review contains a discussion of various turbulence closure models, lists of available two- and three-dimensional hydrodynamic computer codes, code selection guides and case study examples.

The only case study in Part 4 which falls within the realm of multi-dimensional hydrodynamic modeling is 11.5 Neleus (Potomac Residual Chlorine Model). This is a two-dimensional, depth-averaged, finite element model of the upper, fresh water, tidal portion of the Potomac. The case study is deficient in not providing a list of references. The two-dimensional model grid shown in Fig. 11-13 consists of more than 1,100 elements covering a 15-mile portion of the river. Calibration of the model for the 1980 dye study (Fig. 11-14) shows reasonably good agreement. In general, the model is well-suited to provide information on residual chlorine levels.

The group of case studies in Part 4 is deficient in not providing an example of a two-dimensional, laterally-averaged hydrodynamic model. This type of model is well-suited to estuaries that exhibit some degree of salinity of temperature stratification over the depth. Bloss et al (1988) describes the application of a two-dimensional, laterally-averaged hydrodynamic and salinity model to the Trave estuary in Germany. A long-term simulation of 85 days reproduced total mixing events and strong stratification. The model showed good agreement with extensive field data. A similar 2-D model study of stratification and wind-induced destratification in Chesapeake Bay has been reported by Blumberg and Goodrich (1990).

One-dimensional hydrodynamic and salinity models are in an advanced state of development. These cross-sectionally averaged models are applicable to well-mixed estuaries - those having strong tidal regimes and relatively small fresh water inflows. The Delaware and Hudson estuaries are examples of reasonably well-mixed estuaries.

Case study 12.0 (MIT-Dynamic Network Model) applied to the Manasquan River in New Jersey is a good example of a one-dimensional hydrodynamic and salinity model. Longitudinal dispersion is modeled as a function of magnitude of the local salinity gradient and the degree of vertical stratification. Thus this model is able to track longitudinal salinity changes due to variations in fresh water inflow. (Thatcher and Harleman, 1981).

The remaining case studies of Part 4 are 11.3 (Dynamic Estuary Model) applied to the upper portion of the Potomac estuary and 13.0 (RECEIV-II-EPA) applied to the Calcasieu Estuary. These models are pseudo one-dimensional tidal models employing a link-mode schematization. Tidal motion is represented, but the models do not include hydrodynamic and salinity interactions. The primary disadvantage of this class of models is that dispersion effects are not modeled and therefore must be calibrated using conservative tracers. A characteristic of this class of model is their inability to simulate the steepest portion of the longitudinal salinity gradient due to excessive longitudinal numerical dispersion (See Fig. 11-3).

The Calcasieu estuary case study (13.0) states that the model contains no dispersion. The so-called hydrodynamic verification for tidal stages is very poor (See Fig 13.4). This reviewer would not recommend further use of this model for estuarine studies.

14.2.5. Temporal Resolution of Models

The prevalent modeling philosophy throughout this manual (and one that is widely held) is that the temporal resolution of a model should be determined by the time scale of interest to the user of the model output. This usually leads to the conclusion that time steps averaged over a tidal period or longer are desirable. The result is a model far removed from the physics (fluid mechanics) of the relevant transport and mixing process. Thus the modeler is required to "select" multi-dimensional dispersion coefficients which must be "adjusted" by calibration to inadequate data. This approach is based on the mistaken assumption that there is some inherent law stating that there must a correspondence between the time scale of the model input (and the computational time scale) and that of the output.

An alternative approach is to take advantage of the powerful hydrodynamic computational tools that are available in one, two or three dimensions. These require temporal resolution at the intratidal level. The question then arises as to how to interact the small time step hydrodynamic model with the longer time step water quality model (This is the subject of a separate discussion below). The philosophical point is that model output can be averaged temporally in any way that is desired to produce a result at the time scale of interest to the user. In other words, one should not average the input in order to produce an averaged output.

14.2.6. *Time and Space Scales for Interfacing Hydrodynamic and Water Quality Models*

The rational methodology for waste load allocation makes use of water quality models that are capable of predicting the response of a water body to various loading scenarios. We are increasingly called upon to model water bodies that have high degrees of temporal and spatial complexity. Examples are unsteady, strongly advective flow systems with density stratification due to temperature, suspended and/or dissolved substances. Such systems are at least two-dimensional and more often three-dimensional in nature.

There exists, on one hand, a number of 2- and 3-dimensional models that include baroclinic (i.e., stratification) effects and sophisticated hydrodynamic turbulence closure components. On the other hand, there are a number of ecologically sound, multi-parameter water quality models. These two types of models have evolved independently of one another through the efforts of hydrodynamicists and aquatic scientists. A great deal of research support has gone into these separate model development efforts. However, there has been little effort directed to the crucial problem of interfacing or coupling of hydrodynamic transport and water quality models. The coupling problem arises because of the following dichotomy.

The dynamic nature of multi-dimensional hydrodynamic models and the associated numerical stability requirements usually dictate a small spatial grid and a computational time step of the order of minutes. Water quality models typically involve longer time scales ranging from a day in the case of nutrient recycling in the water column to months or years for sediment-water column interactions. There is an obvious disinclination to interface water quality models at the small spatial and temporal resolution of the hydrodynamic model because of the enormous computational burden. Yet there do not exist generic guidelines for interfacing water quality models at larger spatial and temporal increments.

The state of the art of interfacing hydrodynamic and water quality models has evolved in two directions. The first makes use of large boxes where, because of the large spatial grid, it is impossible to apply numerical hydrodynamic models. The user is then faced with the problem of empirically calibrating transport and mixing to an observed distribution such as temperature or dissolved solids. It is impossible to carry out such "large box" calibrations in stratified, strongly time-varying, multidimensional systems.

The second interfacing approach averages the advective and diffusive output of the short time step hydrodynamic model over larger spatial grids and time periods (e.g., 24 hours) that are thought to be appropriate to the water quality model. The problem is that important advective and diffusive information from the hydrodynamic model is lost in direct proportion to the length of the spatial and temporal averaging period. There are no quantitative guidelines for multi-dimensional models to indicate the extent of information loss by averaging. Therefore, we are again faced with the necessity of difficult empirical calibration procedures.

A number of studies have addressed the hydrodynamic-water quality interfacing problem in the context of one-dimensional lake and reservoir models: Ford and Thornton (1979), Imboden et al. (1983), Wang and Harleman (1983), and Shanahan and Harleman (1984). Systematic studies of interfacing for time-varying, multi-dimensional, stratified water bodies are now underway in connection with the EPA/COE Chesapeake Bay modeling program.

14.2.7. *Water Quality-Eutrophication Models*

The water quality components of most of the waste load allocation models in Part 4 are fairly similar in that they model BOD, DO, ammonia, nitrite, nitrate orthophosphate and chlorophyll. In some case, more than one class of algae are included, and some models include zooplankton although data for this component is usually sparse or non-existent.

Three important waste load allocation and management issues are virtually ignored by the water quality-eutrophication models presented in Part 4. They are:

(a) The question of nitrogen or phosphorus limitation in the eutrophication process together with the role of point versus non-point sources as sources of N and P is of crucial importance in waste load allocation. The issue of major investments in advanced waste treatment plants as opposed to control of agricultural fertilizer runoff depends on the model's ability to deal with nutrient limitation kinetics. The problem is complicated by the fact that most estuaries include upstream fresh water portions as well as the downstream salinity intrusion region. Algal species and nutrient preferences may shift between the fresh-salt water zones of an estuary.

(b) A significant number of estuaries experience summer anoxic conditions in deep bottom zones. Very low or zero dissolved oxygen is known to trigger major increases in the release of nutrients from the bottom sediment to the overlying water. Eutrophication models applied to estuaries having low DO problems must have the ability to simulate the vertical stratification and vertical mixing processes that affect vertical oxygen transport and dissolved oxygen gradients and benthic nutrient fluxes.

(c) The determination of the time scale at which an estuary responds to changes in waste load inputs depends on how sediment-water column interactions are modeled. Waste load (nutrient) inputs generally result in algal production in the upper euphotic zone. Dead algae sink and are incorporated as organic material into bottom sediment. Sediment diagenesis occurs in the sediment and results in nutrient fluxes and sediment oxygen demand. The rate at which the sediment diagenesis occurs controls the rate at which the estuary responds to loading changes. Important papers in this modeling area are contained in Hatcher (1986).

Attention should be given in this document to a report prepared by ASCE Task Committee on the Verification of Models of Hydrologic Transport and Dispersion (Ditmars et al,1987). The objective of the report is to identify, collate, and define the procedures required for evaluation of performance of an analytical or numerical surface water model. The essential elements are: identification of the problem; relationship of the model to the problem; solution scheme examination, model response studies, model calibration; and model validation. Literature examples are used to define the techniques that have been used to address each of the elements above. Emphasis in the six elements is placed on moving the evaluation of models, particularly those in journal publication, towards more quantitative or objective measures of calibration and validation.

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14.3.1. Introduction

This assessment of selected case studies of estuarine modeling was prefaced by an opportunity afforded by the Environmental Protection Agency to review drafts of the proposed technical guidance manual for waste load allocation in estuarine systems. It draws on this background to some extent, but is based primarily on the experience of the reviewer in developing and applying mathematical models as tools in support of decision making in water quality management, much of which has been concerned with estuaries. Naturally, the views expressed here are reflective of this experience and are uniquely those of the reviewer, for which he takes full responsibility.

Before examining the specifics of the selected case studies, it is appropriate to identify a few of the characteristics or attributes to the modeling process that need special attention in bringing models to a level of effective application as decision support tools. Among the more important of these are the following:

- Specific goals or objectives of users to be met by the use of models and related decision support capabilities.
- Basic data and information required for construction, calibration, and verification of model(s).
- Temporal and spatial scales appropriate to the intended use of model(s).
- Hydrodynamics input to water quality models.
- Model structure and complexity.
- Calibration and verification.
- Some brief comments concerning each of these will provide a reference for the succeeding case study critiques.
- Goals and Objectives.

In the present context, models are to serve as useful tools in the decision process, i.e. they are to enable a decision maker to make better, more defensible choices among alternatives for waste load allocation. Although some users would like to use estuarine models in predictive modes, this is rarely feasible at the present state of the art. Most of models currently available for water quality simulation are inherently uncertain to a degree that absolute prediction is exceedingly risky. However, after careful calibration and verification estuarine water quality models can usually be applied with confidence in assessment of incremental changes between simulated solutions for different structural or operational alternatives.

14.3.2. Basic Data and Information

The weakest aspect of most modeling projects is the data base. Most often data are gathered without a view to future development or application of a model, and the modeler is forced to adapt to an existing but inadequate body of data. This has prompted some modelers to resort to construction of simple box or statistical models rather than design and implement a data base to serve model application. A well designed data collection program is the best confidence builder for modeling. It should be a continuing activity in any situation where models are to serve future management of estuarine water quality.

14.3.3. Temporal and Spatial Scales

Selection of time and space scales for modeling is an activity that is closely related to definition of objectives. If decisions are to be based on long term (monthly or more) means, then the dynamics of water quality/ecologic processes on a diurnal or tidal basis may not be necessary, although it may still be risky to smooth short term data on these processes, thereby eliminating important information on extremes. Often it is the extreme values, occurring during daily or tidal periods, that are of greatest importance in waste load allocation. Temporal or spatial averaging may be justified in cases where the data are sparse or where the decision process does not require great detail. In today's world of computers the cost of simulation is fast becoming a non issue, that is, the degree of temporal or spatial discretization is virtually at the discretion of the user. If model detail is required, it is more likely to be controlled by the availability of data for calibration and verification than computation cost.

14.3.4. Hydrodynamics

In the judgement of this reviewer inadequate description of advective transport is probably the most common cause of poor calibration and verification in water quality models. This need not be the case, however, since good hydrodynamic models exist for virtually all types of estuarine systems, from simple one-dimensional channel networks to complex stratified estuaries of broad lateral extent where three-dimensional representation is required. Most of these models are relatively easy to calibrate and verify, compared to their water quality companions, and produce descriptions of water levels and current structure that are useful for "driving" water quality simulators.

It is good to recognize in this connection that there is an important trade off between improving simulation of advective processes, which entails additional spatial and temporal detail, and depending on empirically derived dispersive fluxes to describe transport of pollutants. Model simplification usually means greater uncertainty, which in water quality simulation is usually manifest in empirical dispersion coefficients which represent the aggregate effects of many ill-defined quantities.

14.3.5. Model Structure and Complexity

The trend in water quality modeling has generally been toward increasing complexity, i.e. more state variables and an even greater number of additional rate constants, coefficients, etc. While this is a commendable trend in the sense of improved understanding of the aquatic system, it also introduces increased uncertainty in model output, due in major part to the inherent uncertainties in the parameters that have to be estimated or empirically determined. There is probably a level of detail that is "best" for a given situation, somewhere between a simple black box and the detailed model, which produces the most reliable result from the decision maker's viewpoint. Uncertainty analysis, e.g. first order error analysis, Monte Carlo simulation, etc., may provide some guidance as to best structure for the model in relation to decision goals.

14.3.6. Calibration and Verification

Although modeling implicitly requires comparison of simulation and prototype observations, and most modelers comply with the two step process, the practice is still largely judgmental. There are comparatively few examples of rigorous objective assessment of model reliability. There is a need for formalizing calibration and verification procedures, perhaps along the lines of the uncertainty analysis approach suggested above.

14.3.7. Case Study Review

The five case studies were ostensibly selected for the diversity of modeling approaches to characterization of estuarine water quality. They were chosen also, so it appears, to represent a range of difficulties encountered in applying existing models to actual estuaries and further to illustrate varying degrees of success in overcoming these difficulties. No ideal examples are provided, since none actually exist. However, while those chosen for this review can fairly be regarded as instructive of some of the problems encountered in the real world of water quality modeling, they may not be as exemplary of estuarine modeling per se as one would like. In two of these cases, as we shall see, there is reasonable doubt that the systems modeled can even be categorized as estuaries within the definitions provided in the technical guidance manual.

Yet, the several case studies do represent applications of a number of different models and it is useful to examine these for comparative purposes. Because the type of estuary often dictates the structure of the model most suitable for simulation of its hydrodynamic and water quality behavior, this reviewer has chosen to organize his critique according to the specific geographic situation.

Case Study 1 - Saginaw Bay

This is a non-estuary, at least in so far as classical definitions apply. The major difficulties here appear to be most likely associated with characterization of transport rates, both advective and dispersive. Although it is acknowledged that "water levels and flow directions of the Bay change" there is no explicit treatment of the hydromechanical behavior of the water body. Admittedly, this is not a trivial undertaking from a modeling viewpoint, although there are some excellent examples of two- and three-dimensional circulation models for the Great Lakes that would probably be suitable for Saginaw Bay.

The complexity of the ecosystem dynamics represented in this model and the rough "box" configuration of the embayment, both suggest a greater interest in ecosystem kinetics than in the practical problem of waste load allocation. Both of these aspects, simplicity in the one extreme (5 boxes) and complexity in the other (18 plus compartments), lead to increased uncertainty in the results of simulations. This reviewer suggests that perhaps a better result from the point of view of the decision maker might have been obtained with a somewhat more rigorous description of lake circulation and some aggregation in ecosystem compartments. The trends indicated by the results shown seem hardly sufficient for decision purposed in light of apparent uncertainties in model parameters and field data.

This is a case where it seems that the third spatial dimension could be especially important in the model. To what degree does stratification of water quality variables play a role in determining primary productivity? What about vertical advection and dispersion? It is not clear that changes along the vertical axis are important considerations in this case study, although they should be.

In summary, Saginaw Bay is not an estuary, so as a case study of estuarine modeling this example leaves much to be desired. Nevertheless, it is instructive in that it illustrates the tradeoff between hydrodynamic circulation and dispersion as driving forces in water quality modeling, as opposed to increased complexity in ecosystem description. However, because of the greatly increased data requirement that accompanies the introduction of more state variables, such a model may not be the most cost effective from the decision viewpoint. Notwithstanding this argument, it may still be a great learning tool. This is probably its most important attribute.

Case Study 2 - Potomac Estuary

Here we deal with a real estuary, but only partially. The focus in this example of the application of the Dynamic Estuary Model (DEM) and the Potomac Eutrophication Model (PEM) is on the upper "fresh water" section of the estuary, where the effects of tidal oscillation are minimal. In this region dispersive effects induced by the tide (which is of rather small amplitude, anyway) are probably negligible and stratification is unlikely to be a significant consideration.

DYNAMIC ESTUARY MODEL

A redeeming feature of the DEM application is that it does address directly the hydrodynamics of the estuarine system, producing time-variant water levels, velocities, and discharges as output of a hydrodynamic model, which are, in turn, utilized in a separate water quality model to describe the fate of pollutants in the estuary. A limitation of the model(s) is that the basic configuration is one-dimensional, that is, flows are directionally constrained. Pseudo two-dimensional representations are possible for shallow vertically mixed embayments, but circulations for such systems should be regarded as rough approximations.

Calibration and verification of the hydrodynamic model was achieved in a straight forward manner. Extensive experience with this model in branching channel estuarine systems, like the Sacramento-San Joaquin Delta for which it was originally developed, indicate that it is easy to calibrate and gives a good account of tidal effects over a wide range of boundary conditions.

The problem of calibrating the DEM for chlorides along the axis of the estuary is attributed to numerical mixing, a consequence of the solution procedure. Despite this difficulty the model appears to give fair results at the far field level. The practice of varying model coefficients from one survey to the next in an arbitrary manner in order to assure the "best fit" is purely subjective and should not be encouraged. If such as procedure is employed, a rational basis for parameter adjustment must be provided. After calibration and verification for the Potomac study the DEM model appears to have been provided with most of the attributes of a useful decision support tool.

POTOMAC EUTROPHICATION MODEL

The PEM has many of the characteristics of QUAL 2E or WASP 4, in that it is essentially a box model for which the boundary fluxes are governed by either a simple hydrologic mass balance or are generated by an external hydrodynamic model like that in DEM, averaged over a tidal cycle. The contention that the "PEM was developed because the existing DEM model focused more on spatial resolution than on the kinetic complexities of eutrophication" implies that spatial resolution is not of consequence in eutrophication and that kinetic complexities could not be accommodated in a modified DEM. This reviewer believes that spatial resolution of the degree afforded by the DEM, as well as the hydrodynamic information such a model provides, are indeed desirable for a eutrophication study such as exemplified by this case. The more detailed kinetics of PEM are, of course, appropriate. However, experience has shown (and another of these case studies illustrates) that the attributes of more complex kinetics need not be at the expense of realistic hydrodynamics.

Spatial resolution and temporal resolution may be dictated in part by the structure of the basic data used to calibrate and verify the model. The practice of aggregating data from several stations and smoothing over time seems in this case to be consistent with a "regional and seasonal focus," but it tends to ignore local and short term events which are often of major concern in setting goals for wastewater management. It also presents problems in calibration and verification, as evidenced in some of the examples given.

The post audit experience, in which the model was unable to predict the magnitude or spatial extent of the 1983 blue-green algae bloom, appears to confirm a need for improved resolution and extension of the model. It is credit to the model developers that the model has been periodically revised to improve its capability as a management tool.

NELEUS - CHLORINE MODEL

The problem presented in modeling the fate of chlorine in the Potomac Estuary is properly addressed with a two-dimensional finite element model, capable of representing the irregular configuration of the water body and providing the essential spatial detail. It is unfortunate that field data were insufficient for thorough calibration, but experience with such models has shown that hydrodynamics can be closely simulated, even for very complex geometries and unsteady boundary conditions.

The water quality model in this package is driven by the hydrodynamic model, but with the added requirement of estimating lateral and longitudinal dispersion coefficients. Again, model calibration was not carried to a satisfactory level, due in major part to inadequate field data. There is insufficient foundation for selection of either dispersion coefficients or the decay rate for chlorine, hence the models at this stage are of questionable use for decision purposes, despite their intrinsic potentials.

The important lesson of this case study is to provide an adequate data base for complete calibration and verification of both hydrodynamic and water quality models.

Case Study - Manasquan Estuary

This case, among all those presented, is probably the most balanced in the treatment of hydrodynamics and water quality, and in calibration and verification methodology. Unfortunately, the MIT-Dynamic Network Model (MIT-DNM) did not reach the stage of actual application as a management tool, so its performance cannot be fully assessed.

The calibration-verification sequence of hydrodynamics/conservative tracer (salinity)/nonconservative water quality is representative of good modeling practice. Because the model is one-dimensional and only a rough approximation of the estuary, it is necessary to utilize an empirically derived dispersion coefficient as a calibration parameter. While the functional relationship between this parameter and geometric and hydraulic properties of the estuary appears well founded in theory and experiment it is nevertheless unique for a particular estuarine system, e.g. constant K and m. It purports to account for factors that cannot be adequately represented in a one dimensional model with such a coarse segmentation, e.g. advective dispersion and stratification. Dependence on this uncertain calibration parameter could probably be reduced by some additional detail in spatial characterization of the estuary.

The relatively unsatisfactory results of water quality calibration point to a need for improving the data base, particularly the pattern of nutrient loading on the estuary. It seems unlikely that the model will become a useful tool for waste load allocation to the Manasquan Estuary until this additional data is developed.

Case Study - Calcasieu River Estuary

This study was allegedly selected in part because it represents the application of a so-called "canned" model supported by EPA. This reviewer disagrees with the implication that such models, exemplified also by such well documented and supported models as QUAL 2E, SWMM, DEM, WASP 4, HEC 5Q, TABS II, etc. are likely to lead to the kind of difficulties encountered in modeling the Calcasieu River Estuary. It is the responsibility of the modeler to select the most appropriate modeling approach for the particular situation. Most often the modeler is well advised to begin with a package that is well documented (as are those cited above) and for which there is a considerable body of experience in adapting to new conditions. If what is available proves to be unsuitable it can be modified, as in this case, or a completely new model can be devised. The test of its capability will be in the processes of calibration and verification.

The principal difficulty with the Calcasieu estuary is that it is so complex that virtually no model existing at the time of the study was fully equal to the task. The tortuous looping and branching channel configuration might at first appear to be a candidate for RECEIV–II, since the model was designed originally for such systems. However, this model assumes vertical homogeneity where the Calcasieu system includes many sections which are stratified. The system also includes very broad channel reaches and embayments, even lakes, which are not well represented hydrodynamically by the pseudo two-dimensional network approximation possible with RECEIV–II. The existence of stratified lakes within the system suggests the need for a model capable of dealing with hydrodynamics in one, two or three dimensions, depending on the local conditions. A finite element approach is probably the most feasible at present, although in fairness to the modelers of the Calcasieu estuary it is acknowledged that such a model was not available at the time of the study.

Hydrodynamic calibration/verification for this study was described as "good," although in certain instances elevation differences between model and prototype were large enough to indicate that system storage was not well simulated, e.g. 1978. Water quality calibration/verification was fair at best, a result attributed by the modeler to inadequate input information and dynamics. Here again the complexity of the system and the water quality model, with its large number of parameters, probably preclude a good result. Future modeling efforts for this estuary should be directed to improving hydrodynamic simulation and estimates of waste loads.

14.3.8. Concluding Comment

This selection of case studies illustrates most of the problems encountered in modeling of water quality in estuarine systems. Among the lessons to be learned from these experiences, the following appear to this reviewer to be the more significant in directing future modeling efforts.

1. There is no substitute for hard data from the field. Data collection programs should be designed with model requirements in mind.

2. Water quality models of estuarine systems are driven by hydrodynamics. More attention needs to be given

to the hydrodynamic driver as an integral part of the modeling package. In particular, effects of stratification should be explicitly modeled.

3. Complexity may lead to more uncertainty in model results. Adding more compartments may improve fundamental understanding of important mechanisms, but it requires more data and does not necessarily lead to better decisions.

4. Models should be designed and applied as tools to support decisions by non-modelers. Output should be readily interpretable by decision makers.

5. Calibration/verification is still largely a subjective process. Criteria for acceptance of a verified model should be developed and related to the intended use of the model in the decision process.