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Reference

Technical Guidance Manual for Performing Waste Load Allocations

Book III
Estuaries

Part 2
Application of Estuarine Waste Load Allocation Models

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TECHNICAL GUIDANCE MANUAL FOR PERFORMING WASTE LOAD ALLOCATIONS

BOOK III: ESTUARIES

Part 2: Application of Estuarine Waste Load Allocation Models

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Glossary

Acute Toxicity[1] - Any toxic effect that is produced within a short period of time, usually 24-96 hours. Although the effect most frequently considered is mortality, the end result of acute toxicity is not necessarily death. Any harmful biological effect may be the result.

Aerobic[1] - Refers to life or processes occurring only in the presence of free oxygen; refers to a condition characterized by an excess of free oxygen in the aquatic environment.

Algae (Alga)[1] - Simple plants, many microscopic, containing chlorophyll. Algae form the base of the food chain in aquatic environments. Some species may create a nuisance when environmental conditions are suitable for prolific growth.

Allochthonous[1]- Pertaining to those substances, materials or organisms in a waterway which originate outside and are brought into the waterway.

Anaerobic[2] - Refers to life or processes occurring in the absence of free oxygen; refers to conditions characterized by the absence of free oxygen.

Autochthonous[1] - Pertaining to those substances, materials, or organisms originating within a particular waterway and remaining in that waterway.

Autotrophic[1] - Self nourishing; denoting those organisms that do not require an external source of organic material but can utilize light energy and manufacture their own food from inorganic materials; e.g., green plants, pigmented flagellates.

Bacteria[1]- Microscopic, single-celled or noncellular plants, usually saprophytic or parasitic.

Benthal Deposit[2] - Accumulation on the bed of a watercourse of deposits containing organic matter arising from natural erosion or discharges of wastewaters.

Benthic Region[1] - The bottom of a waterway; the substratum that supports the benthos.

Benthal Demand[2] - The demand on dissolved oxygen of water overlying benthal deposits that results from the upward diffusion of decomposition products of the deposits.

Benthos[1] - Organisms growing on or associated principally with the bottom of waterways. These include: (1) sessile animals such as sponges, barnacles, mussels, oysters, worms, and attached algae; (2) creeping forms such as snails, worms, and insects; (3) burrowing forms, which include clams, worms, and some insects; and (4) fish whose habits are more closely associated with the benthic region than other zones; e.g., flounders.

Biochemical Oxygen Demand[2] - A measure of the quantity of oxygen utilized in the biochemical oxidation of organic matter in a specified time and at a specific temperature. It is not related to the oxygen requirements in chemical combustion, being determined entirely by the availability of the material as a biological food and by the amount of oxygen utilized by the microorganisms during oxidation. Abbreviated BOD.

Biological Magnification[1] - The ability of certain organisms to remove from the environment and store in their tissues substances present at nontoxic levels in the surrounding water. The concentration of these substances becomes greater each higher step in the food chain.

Bloom[1] - A readily visible concentrated growth or aggregation of minute organisms, usually algae, in bodies of water.

Brackish Waters[1] - Those areas where there is a mixture of fresh and salt water; or, the salt content is greater than fresh water but less than sea water; or, the salt content is greater than in sea water.

Channel Roughness[2] - That roughness of a channel, including the extra roughness due to local expansion or contraction and obstacles, as well as the roughness of the stream bed proper; that is, friction offered to the flow by the surface of the bed of the channel in contact with the water. It is expressed as roughness coefficient in the velocity formulas.

Chlorophyll[1] - Green photosynthetic pigment present in many plant and some bacterial cells. There are seven known types of chlorophyll; their presence and abundance vary from one group of photosynthetic organisms to another.

Chronic Toxicity[1] - Toxicity, marked by a long duration, that produces an adverse effect on organisms. The end result of chronic toxicity can be death although the usual effects are sublethal; e.g., inhibits reproduction, reduces growth, etc. These effects are reflected by changes in the productivity and population structure of the community.

Coastal Waters[1] - Those waters surrounding the continent which exert a measurable influence on uses of the land and on its ecology. The Great Lakes and the waters to the edge of the continental shelf.

Component Tide[2] - Each of the simple tides into which the tide of nature is resolved. There are five principal components; principal lunar, principal solar, N_2, K, and O. There are between 20 and 30 components which are used in accurate predictions of tides.

Coriolis Effect[2] - The deflection force of the earth's rotation. Moving bodies are deflected to the right in the northern hemisphere and to the left in the southern hemisphere.

Datum[2] - An agreed standard point or plane of state elevation, noted by permanent bench marks on some solid immovable structure, from which elevations are measured or to which they are referred.

Density Current[2] - A flow of water through a larger body of water, retaining its unmixed identity because of a difference in density.

Deoxygenation[2] - The depletion of the dissolved oxygen in a liquid either under natural conditions associated with the biochemical oxidation of organic matter present or by addition of chemical reducing agents.

Diagenetic Reaction - Chemical and physical changes that alter the characteristics of bottom sediments. Examples of chemical reactions include oxidation of organic materials while compaction is an example of a physical change.

Dispersion[2] - (1) Scattering and mixing. (2) The mixing of polluted fluids with a large volume of water in a stream or other body of water.

Dissolved Oxygen[2] - The oxygen dissolved in water, wastewater, or other liquid, usually expressed in milligrams per liter, or percent of saturation. Abbreviated DO.

Diurnal[2] - (1) Occurring during a 24-hr period; diurnal variation. (2) Occurring during the day time (as opposed to night time). (3) In tidal hydraulics, having a period or cycle of approximately one tidal day.

Drought[2] - In general, an extended period of dry weather, or a period of deficient rainfall that may extend over an indefinite number of days, without any quantitative standard by which to determine the degree of deficiency needed to constitute a drought. Qualitatively, it may be defined by its effects as a dry period sufficient in length and severity to cause at least partial crop failure or impair the ability to meet a normal water demand.

Ebb Tide[1] - That period of tide between a high water and the succeeding low water; falling tide.

Enrichment[1] - An increase in the quantity of nutrients available to aquatic organisms for their growth.

Epilimnion[1] - The water mass extending from the surface to the thermocline in a stratified body of water; the epilimnion is less dense that the lower waters and is wind-circulated and essentially homothermous.

Estuary[1] - That portion of a coastal stream influenced by the tide of the body of water into which it flows; a bay, at the mouth of a river, where the tide meets the river current; an area where fresh and marine water mix.

Euphotic Zone[1] - The lighted region of a body of water that extends vertically from the water surface to the depth at which photosynthesis fails to occur because of insufficient light penetration.

Eutrophication[1] - The natural process of the maturing (aging) of a lake; the process of enrichment with nutrients, especially nitrogen and phosphorus, leading to increased production of organic matter.

Firth[1] - A narrow arm of the sea; also the opening of a river into the sea.

Fjord (Fiord)[1] - A narrow arm of the sea between highlands.

Food Chain[1] - Dependence of a series of organisms, one upon the other, for food. The chain begins with plants and ends with the largest carnivores.

Flood Tide[2] - A term indiscriminately used for rising tide or landward current. Technically, flood refers to current. The use of the terms "ebb" and "flood" to include the vertical movement (tide) leads to uncertainty. The terms should be applied only to the horizontal movement (current).

Froude's Number[2] - A numerical quantity used as an index to characterize the type of flow in a hydraulic structure that has the force of gravity (as the only force producing motion) acting in conjunction with the resisting force of inertia. It is equal to the square of characteristic velocity (the mean, surface, or maximum velocity) of the system, divided by the product of a characteristic linear dimension, such as diameter or expressed in consistent units so that the combinations will be dimensionaless. The number is used in open-channel flow studies or in cases in which the free surface plays an essential role in influencing motion.

Heavy Metals[2] - Metals that can be precipitated by hydrogen sulfide in acid solution, for example, lead, silver, gold, mercury, bismuth, copper.

Heterotrophic[1] - Pertaining to organisms that are dependent on organic material for food.

Hydraulic Radius[2] - The right cross-sectional area of a stream of water divided by the length of that part of its periphery in contact with its containing conduit; the ratio of area to wetted perimeter. Also called hydraulic mean depth.

Hydrodynamics[2] - The study of the motion of, and the forces acting on, fluids.

Hydrographic Survey[2] - An instrumental survey made to measure and record physical characteristics of streams and other bodies of water within an area, including such things as location, areal extent and depth, positions and locations of high-water marks, and locations and depths of wells.

Inlet[1] - A short, narrow waterway connecting a bay, lagoon, or similar body of water with a large parent body of water; an arm of the sea, or other body of water, that is long compared to its width, and that may extend a considerable distance inland.

Inorganic Matter[2] - Mineral-type compounds that are generally non-volatile, not combustible, and not biodegradable. Most inorganic-type compounds, or reactions, are ionic in nature, and therefore, rapid reactions are characteristic.

Lagoon[1] - A shallow sound, pond, or channel near or communicating with a larger body of water.

Limiting Factor[1] - A factor whose absence, or excessive concentration, exerts some restraining influence upon a population through incompatibility with species requirements or tolerance.

Manning Formula[2] - A formula for open-channel flow, published by Manning in 1890, which gives the value of c in the Chezy formula.

Manning Roughness Coefficient[2] - The roughness coefficient in the Manning formula for determination of the discharge coefficient in the Chezy formula.

Marsh[1] - Periodically wet or continually flooded area with the surface not deeply submerged. Covered dominantly with emersed aquatic plants; e.g., sedges, cattails, rushes.

Mean Sea Level[2] - The mean plane about which the tide oscillates; the average height of the sea for all stages of the tide.

Michaelis-Menton Equation[2] - A mathematical expression to describe an enzyme-catalyzed biological reaction in which the products of a reaction are described as a function of the reactants.

Mineralization[2] - The process by which elements combined in organic form in living or dead organisms are eventually reconverted into inorganic forms to be made available for a fresh cycle of plant growth. The mineralization of organic compounds occurs through combustion and through metabolism by living animals. Microorganisms are ubiquitous, possess extremely high growth rates and have the ability to degrade all naturally occurring organic compounds.

Modeling[2] - The simulation of some physical or abstract phenomenon or system with another system believed to obey the same physical laws or abstract rules of logic, in order to predict the behavior of the former (main system) by experimenting with latter (analogous system).

Monitoring[2] - Routine observation, sampling and testing of designated locations or parameters to determine efficiency of treatment or compliance with standards or requirements.

Mouth[2] - The exit or point of discharge of a stream into another stream or a lake, or the sea.

Nautical Mile[2] - A unit of distance used in ocean navigation. The United States nautical mile is defined as equal to one-sixteenth of a degree of a great circle on a sphere with a surface equal to the surface of the earth. Its value, computed for the Clarke spheroid of 1866, is 1,853.248 m (6,080.20ft). The International nautical mile is 1,852 m (6,070.10 ft).

Nanoplankton[2] - Very minute plankton not retained in a plankton net equipped with no. 25 silk bolting cloth (mesh, 0.03 to 0.04 mm.).

Neap Tides[1] - Exceptionally low tides which occur twice each month when the earth, sun and moon are at right angles to each other; these usually occur during the moon's first and third quarters.

Neuston[2] - Organisms associated with, or dependent upon, the surface film (air-water) interface of bodies of water.

Nitrogenous Oxygen Demand (NOD)[2] - A quantitative measure of the amount of oxygen required for the biological oxidation of nitrogenous material, such as ammonia nitrogen and organic nitrogen, in wastewater; usually measured after the carbonaceous oxygen demand has been satisfied.

Nutrients[1] - Elements, or compounds, essential as raw materials for organism growth and development; e.g., carbon, oxygen, nitrogen, phosphorus, etc.

Organic[1] - Refers to volatile, combustible, and sometimes biodegradable chemical compounds containing carbon atoms (carbonaceous) bonded together and with other elements. The principal groups of organic substances found in wastewater are proteins, carbohydrates, and fats and oils.

Oxygen Deficit[1] - The difference between observed oxygen concentration and the amount that would theoretically be present at 100% saturation for existing conditions of temperature and pressure.

Pathogen[1] - An organism or virus that causes a disease.

Periphyton (Aufwuchs)[1] - Attached microscopic organisms growing on the bottom, or other submersed substrates, in a waterway.

Photosynthesis[1] - The metabolic process by which simple sugars are manufactured from carbon dioxide and water by plant cells using light as an energy source.

Phytoplankton[1] - Plankton consisting of plant life. Unattached microscopic plants subject to movement by wave or current action.

Plankton[1] - Suspended microorganisms that have relatively low powers of locomotion, or that drift in the water subject to the action of waves and currents.

Quality[2] - A term to describe the composite chemical, physical, and biological characteristics of a water with respect to it's suitability for a particular use.

Reaeration[2] - The absorption of oxygen into water under conditions of oxygen deficiency.

Respiration[1] - The complex series of chemical and physical reactions in all living organisms by which the energy and nutrients in foods is made available for use. Oxygen is used and carbon dioxide released during this process.

Roughness Coefficient[2] - A factor, in the Chezy, Darcy-Weisbach, Hazen-Williams, Kutter, Manning, and other formulas for computing the average velocity of flow of water in a conduit or channel, which represents the effect of roughness of the confining material on the energy losses in the flowing water.

Seiche[1] - Periodic oscillations in the water level of a lake or other landlocked body of water due to unequal atmospheric pressure, wind, or other cause, which sets the surface in motion. These oscillations take place when a temporary local depression or elevation of the water level occurs.

Semidiurnal[2] - Having a period or cycle of approximately one half of a tidal day. The predominating type of tide throughout the world is semidiurnal, with two high waters and two low waters each tidal day.

Slack Water[2] - In tidal waters, the state of a tidal current when its velocity is at a minimum, especially the moment when a reversing current changes direction and its velocity is zero. Also, the entire period of low velocity near the time of the turning of the current when it is too weak to be of any practical importance in navigation. The relation of the time of slack water to the tidal phases varies in different localities. In some cases slack water occurs near the times of high and low water, while in other localities the slack water may occur midway between high and low water.

Spring Tide[1] - Exceptionally high tide which occurs twice per lunar month when there is a new or full moon, and the earth, sun, and moon are in a straight line.

Stratification (Density Stratification)[1] - Arrangement of water masses into separate, distinct, horizontal layers as a result of differences in density; may be caused by differences in temperature, dissolved or suspended solids.

Tidal Flat[1] - The sea bottom, usually wide, flat, muddy and nonproductive, which is exposed at low tide. A marshy or muddy area that is covered and uncovered by the rise and fall of the tide.

Tidal Prism[2] - (1) The volume of water contained in a tidal basin between the elevations of high and low water. (2) The total amount of water that flows into a tidal basin or estuary and out again with movement of the tide, excluding any fresh-water flows.

Tidal Range[2] - The difference in elevation between high and low tide at any point or locality.

Tidal Zone (Eulittoral Zone, Intertidal Zone)[1] - The area of shore between the limits of water level fluctuation; the area between the levels of high and low tides.

Tide[1] - The alternate rising and falling of water levels, twice in each lunar day, due to gravitational attraction of the moon and sun in conjunction with the earth's rotational force.

Tide Gage[2] - (1) A staff gage that indicates the height of the tide. (2) An instrument that automatically registers the rise and fall of the tide. In some instruments, the registration is accomplished by printing the heights at regular intervals; in others by a continuous graph in which the height of the tide is represented by ordinates of the curve and the corresponding time by the abscissae.

Toxicant[1] - A substance that through its chemical or physical action kills, injures, or impairs an organism; any environmental factor which, when altered, produces a harmful biological effect.

Water Pollution[1] - Alteration of the aquatic environment in such a way as to interfere with a designated beneficial use.

Water Quality Criteria[1] - A scientific requirement on which a decision or judgement may be based concerning the suitability of water quality to support a designated use.

Water Quality Standard[1] - A plan that is established by governmental authority as a program for water pollution prevention and abatement.

Zooplankton[2] - Plankton consisting of animal life. Unattached microscopic animals having minimal capability for locomotion.

1Rogers, B.G., Ingram, W.T., Pearl, E.H., Welter, L.W. (Editors). 1981, Glossary, Water and Wastewater Control Engineering, Third Edition, American Public Health Association, American Society of Civil Engineers, American Water Works Association, Water Pollution Control Federation.

2Matthews, J.E., 1972, Glossary of Aquatic Ecological Terms, Manpower Development Branch, Air and Water Programs Division, EPA, Oklahoma.

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Executive Summary

The Technical Guidance Manual for Performing Waste Load Allocations, Book III: Estuaries is the third in a series of manuals providing technical information and policy guidance for the preparation of waste load allocations (WLAs) that are as technically sound as current state of the art permits. The objective of such load allocations is to ensure that water quality conditions that protect designated beneficial uses are achieved. This book provides technical guidance for performing waste load allocations in estuaries.

PART I: ESTUARIES AND WASTE LOAD ALLOCATION MODELS

Introduction

Estuaries are coastal bodies of water where fresh water meets the sea. Most rivers and their associated pollutant loads eventually flow into estuaries. The complex loading, circulation, and sedimentation processes make water quality assessment and waste load allocation in estuaries difficult. Transport and circulation processes in estuaries are driven primarily by river flow and tidal action. As a consequence of its complex transport processes, estuaries cannot be treated as simple advective systems such as many rivers.

Wastewater discharges into estuaries can affect water quality in several ways, both directly and indirectly. In setting limits on wastewater quantity and quality, the following potential problems should be assessed: salinity, sediment, pathogenic bacteria, dissolved oxygen depletion, nutrient enrichment and overproduction, aquatic toxicity, toxic pollutants and bioaccumulation and human exposure.

A WLA provides a quantitative relationship between the waste load and the instream concentrations or effects of concern as represented by water quality standards. During the development of a WLA, the user combines data and model first to describe present conditions and then to extrapolate to possible future conditions. The WLA process sequentially addresses the topics of hydrodynamics, mass transport, water quality kinetics, and for some problems, bioaccumulation and toxicity.

For each of the topics addressed in a modeling study, several steps are applied in an iterative process: problem identification, model identification, initial model calibration, sensitivity analysis, model testing, refinement, and validation.

After the WLAs have been put into effect, continued monitoring, post-audit modeling and refinement should lead to more informed future WLAs.

Overview of Processes Affecting Estuarine Water Quality

The estuarine waste load allocation process requires a fundamental understanding of the factors affecting water quality and the representation of those processes in whatever type of model is applied (conceptual or mathematical) in order to determine the appropriate allocation of load. Insight into processes affecting water quality may be obtained through examination of the schemes available for their classification. Estuaries have typically been classified based on their geomorphology and patterns of stratification and mixing. However, each estuary is to some degree unique and it is often necessary to consider the fundamental processes impacting water quality.

To determine the fate and affects of water quality constituents it is necessary first to determine processes impacting their transport. That transport is affected by tides, fresh water inflow, friction at the fluid boundaries and its resulting turbulence, wind and atmospheric pressure, and to a lesser degree (for some estuaries) the effects of the earth's rotation (Coriolis force). The resulting transportation patterns may be described (determined from field studies) in waste load allocation studies, or, as is becoming more frequently the case, estimated using hydrodynamic models. Hydrodynamic models are based on descriptions of the processes affecting circulation and mixing using equations based on laws of conservation of mass and momentum. The fundamental equations generally include: (A) the conservation of water mass (continuity), (B) conservation of momentum, and (C) conservation of constituent mass.

An important aspect of estuarine WLA modeling often is the capability to simulate sediment transport and sediment/water interactions. Sediments not only affect water transparency, but can carry chemicals such as nutrients and toxic substances into receiving waters. Unlike rivers, which have reasonably constant water quality conditions, the large changes in salinity and pH in an estuary directly affect the transport behavior of many suspended solids. Many colloidal particles agglomerate and settle in areas of significant salinity gradients. Processes impacting sediment transport include settling, resuspension, scour and erosion, coagulation and flocculation.

The water quality parameters of interest vary with the objectives of the waste load allocation study, from "conventional pollutants" (e.g. organic waste, dissolved oxygen and nutrients) to toxic organics and trace metals.

The focus of WLA models of conventional pollutants is often DO and biochemical oxygen demand (BOD) as a general measure of the health of the system, or the focus can be primary productivity when eutrophication is the major concern. Conventional WLA models usually include temperature, major nutrients, chemical characteristics, detritus, bacteria, and primary producers. WLA models may include higher trophic levels (i.e. zooplankton and fish) because of higher trophic level effects on other more important variables, such as phytoplankton, BOD and DO. Synthetic organic chemicals include a wide variety of toxic materials whose waste loads are allocated based upon threshold concentrations as well as tolerable durations and frequencies of exposure. These pollutants may ionize and different forms may have differing toxicological effects. The transport of the materials also may be affected by sorption and they can degrade through such processes as volatilization, biodegradation, hydrolysis, and photolysis.

Trace metals may be of concern in many estuaries due to their toxicological effects. The toxicity of trace metals and their transport is affected by their form. Upon entry to a surface water body, metal speciation may change due to complexation, precipitation, sorption, and redox reactions. Metals concentrations are diluted further by additional stream flow and mixing. Physical loss can be caused by settling and sedimentation, whereas a physical gain may be caused by resuspension.

Model Identification and Selection

The first steps in the modeling process are model identification and selection. The goals are to identify the simplest conceptual model that includes all the important estuarine phenomena affecting the water quality problems, and to select the most useful analytical formula or computer model for calculating waste load allocations. During model identification, available information is gathered and organized to construct a coherent picture of the water quality problem. There are four basic steps in model identification: establish study objectives and constraints, determine water quality pollutant interactions, determine spatial extent and resolution, and determine temporal extent and resolution. Following model identification, another important step is advised: perform rapid, simple screening calculations to gain a better understanding of expected pollutant levels and the spatial extent of water quality problems.

The first step in identifying an appropriate WLA model for a particular site is to review the applicable water quality standards and the beneficial uses of the estuary to be protected. Local, state, and federal regulations may contribute to a set of objectives and constraints. The final result of this step should be a clear understanding of the pollutants and water quality indicators, the areas, and the time scales of interest.

After the pollutants and water quality indicators are identified, the significant water quality reactions must be determined. These reactions must directly or indirectly link the pollutants to be controlled with the primary water quality indicators. All other interacting water quality constituents thought to be significant should be included at this point. This can best be done in a diagram or flow chart representing the mass transport and transformations of water quality constituents in a defined segment of water. The final result of this step should be the assimilation of all the available knowledge of a system in a way that major water quality processes and ecological relationships can be evaluated for inclusion in the numerical model description.

The next step is to specify the spatial extent, dimensionality, and scale (or computational resolution) of the WLA model. This may be accomplished by determining the effective dimensionality of the estuary as a whole, defining the boundaries of the study area, then specifying the required dimensionality and spatial resolution within the study area. The effective dimensionality of an estuary includes only those dimensions over which hydrodynamic and water quality gradients significantly affect the WLA analysis. Classification and analysis techniques are available. Specific boundaries of the study area must be established, in general, beyond the influence of the discharge(s) being evaluated. Data describing the spatial gradients of important water quality constituents within the study area should be examined. Dye studies can give important information on the speed and extent of lateral and vertical mixing. It is clear that choice of spatial scale and layout of the model network requires considerable judgment.

The final step in model identification is to specify the duration and temporal resolution of the WLA model. The duration of WLA simulations can range from days to years, depending upon the size and transport characteristics of the study area, the reaction kinetics and forcing functions of the water quality constituents, and the strategy for relating simulation results to the regulatory requirements. One basic guideline applies in all cases - the simulations should be long enough to eliminate the effect of initial conditions on important water quality constituents at critical locations.

The temporal resolution of WLA simulations falls into one of three categories - dynamic, quasi-dynamic, and steady state. Dynamic simulations predict hour to hour variations caused by tidal transport. Quasidynamic simulations predict variations on the order of days to months. The effects of tidal transport are time-averaged. Other forcing functions such as freshwater inflow, pollutant loading, temperature, and sunlight may vary from daily to monthly. Steady state simulations predict monthly to seasonal averages. All inputs are time-averaged. Two schools of thought have persisted regarding the utility of dynamic versus quasidynamic and steady state simulations. For some problems the choice is reasonably clear.

In general, if the regulatory need or kinetic response is on the order of hours, then dynamic simulations are required; if regulatory needs are long term averages and the kinetic response is on the order of seasons to years, then quasidynamic or steady simulations are indicated.

The goal of model selection is to obtain a simulation model that effectively implements the conceptual model identified for the WLA. Models selected for discussion here are general purpose, in the public domain, and available from or supported by public agencies. The selection of an estuarine WLA model need not be limited to the models discussed in this document. Other models that are available to a project or organization should also be considered. The models summarized in this report represent the typical range of capabilities currently available. Estuarine WLA models can be classified as Level I to Level IV according to the temporal and spatial complexity of the hydrodynamic component of the model. Level I includes desktop screening methodologies that calculate seasonal or annual mean pollutant concentrations based on steady state conditions and simplified flushing time estimates. These models are designed to examine an estuary rapidly to isolate trouble spots for more detailed analyses.

Level II includes computerized steady state or tidally averaged quasidynamic simulation models, which generally use a box or compartment-type network to solve finite difference approximations to the basic partial differential equations. Level II models can predict slowly changing seasonal water quality with an effective time resolution of 2 weeks to 1 month. Level III includes computerized one-dimensional (1-d) and quasi two-dimensional (2-d), dynamic simulation models. These real time models simulate variations in tidal heights and velocities throughout each tidal cycle. Their effective time resolution is usually limited to average variability over one week because tidal input parameters generally consist of only average or slowly varying values. The effective time resolution could be reduced to under 1 day given good representation of diurnal water quality kinetics and precise tidal input parameters. The required data and modeling effort are usually not mobilized in standard WLAs.

Level IV consists of computerized 2-d and 3-d dynamic simulation models. Dispersive mixing and seaward boundary exchanges are treated more realistically than in the Level III 1-d models. These models are almost never used for routine WLAs. The effective time resolution of the Level IV models can be less than 1 day with a good representation of diurnal water quality and intratidal variations.

The advantages of Level I and II models lie in their comparatively low cost and ease of application. The disadvantages lie in their steady state or tidally averaged temporal scale. When hydrodynamics and pollutant inputs are rapidly varying, steady state models are difficult to properly calibrate.

The dynamic models (Levels III and IV) have advantages over steady state and tidally averaged models in representing mixing in partially mixed estuaries because advection is so much better represented. The success with which these models can predict transient violations depends upon both the accuracy and resolution of the loading and environmental data, and the model's treatment of short time scale kinetics such as desorption or diurnal fluctuations in temperature, pH, or sunlight. While dynamic models are capable of predicting diurnal and transient fluctuations in water quality parameters, the input data requirements are much greater.

PART II: APPLICATION OF ESTUARINE WASTE LOAD ALLOCATION MODELS

Monitoring Protocols for Calibration and Validation of Estuarine Waste Load Allocation Models

The monitoring data collected in support of a modeling study is used to: (1) determine the type of model application required (e.g. dimensionality, state variables); (2) perturb the model (e.g. loadings, flows); (3) provide a basis for assigning rate coefficients and model input parameters (model calibration); and (4) determine if the model adequately describes the system (model evaluation).

The specific types of data and quantity required will vary with the objectives of the WLA modeling study and the characteristics of the estuary. Data are always required to determine model morphometry, such as depths and volumes (e.g. available from sounding data or navigation charts). Data are also required for transport. Transport within the modeled system may either be specified (measured, e.g. current meters) or computed from hydrodynamic models. Flows into the system must be measured, or in the case of the open boundary, water surface elevations must be determined.

The water quality data required, beyond that needed to quantify transport, will vary depending on how the variables will be used and their anticipated impact on the system. Data requirements will differ if the WLA modeling study is intended for dissolved oxygen, eutrophication or toxics. Concentrations for all pertinent water quality variables should be provided at the model boundaries, providing the perturbation for model predictions, as well as at points within the waterbody to provide a basis for estimating model parameters and evaluating model predictions. Data should be available to determine variations in water quality parameters over space and time.

Planning monitoring studies should be a collaborative effort of participants involved in budgeting, field collection, analysis and processing of data, quality assurance, data management and modeling activities.

Collaboration insures that fundamental design questions are properly stated so that the available resources are used in the most efficient manner possible and that all critical data for modeling are collected. The use of monitoring and modeling in an iterative fashion, wherever possible, is often the most efficient means of insuring that critical data are identified and collected. A rigorous, well documented, quality assurance, quality control (QA/QC) plan should be an integral part of any waste load allocation program.

Model Calibration, Validation, and Use

While models can be run with minimal data, their predictions are subject to large uncertainty. Models are best operated to interpolate between existing conditions or to extrapolate from existing to future conditions, such as in the projection of conditions under anticipated waste loads. The confidence that can be placed on those projections is dependent upon the integrity of the model, and how well the model is calibrated to that particular estuary, and how well the model compares when evaluated against an independent data set (to that used for calibration).

Model calibration is necessary because of the semi-empirical nature of present day (1990) water quality models. Although the waste load allocation models used in estuary studies are formulated from the mass balance and, in many cases, from conservation of momentum principles, most of the kinetic descriptions in the models that describe the change in water quality are empirically derived. These empirical derivations contain a number of coefficients and parameters that are usually determined by calibration using data collected in the estuary of interest.

Calibration alone is not adequate to determine the predictive capability of a model for a particular estuary. To map out the range of conditions over which the model can be used to determine cause and effect relationships, one or more additional independent sets of data are required to determine whether the model is predictively valid. This testing exercise, which also is referred to as confirmation testing, defines the limits of usefulness of the calibrated model. Without validation testing, the calibrated model remains a description of the conditions defined by the calibration data set. The uncertainty of any projection or extrapolation of a calibrated model would be unknown unless this is estimated during the validation procedure.

In addition, the final validation is limited to the range of conditions defined by the calibration and validation data sets. The uncertainty of any projection or extrapolation outside this range also remains unknown. The validation of a calibrated model, therefore, should not be taken to infer that the model is predictively valid over the full range of conditions that can occur in an estuary. For example, a model validated over the range of typical tides and low freshwater inflow may not describe conditions that occur when large inflows and atypical tides occur.

This is especially true when processes such as sediment transport and benthic exchange occur during atypical events but not during the normal, river flow and tidal events typically used to calibrate and validate the model.

Following model calibration and validation, several types of analyses of model performance are of importance. First, a sensitivity analysis provides a method to determine which parameters and coefficients have the greatest impact on model predictions. Second, there are a number of statistical tests that are useful for defining when adequate agreement has been obtained between model simulations and measured conditions in order to estimate the confidence that may be assigned to model predictions. Finally, a components analysis indicates the relative contribution of processes to variations in predicted concentrations. For example, the cause of violations of a dissolved oxygen standard can be determined from the relative contribution of various loads and the effect of sediment oxygen demand, BOD decay, nitrification, photosynthesis, and reaeration.

Once the model is calibrated and validated, it is then used to investigate causes of existing problems or to simulate future conditions to determine effects of changes in waste loads as part of the waste load allocation procedure. Once critical water quality conditions are defined for the estuary, harbor or coastal area of concern, determining the waste assimilative capacity is relatively straightforward. Models are available to relate critical water quality responses to the loads for most problems. However, the definition of critical conditions for estuaries is not straightforward. For streams receiving organic loads, this is a straightforward matter of determining the low flow and high temperature conditions. In estuaries, fresh water, tides, wind, complex sediment transport, and other factors can be important to determining the critical conditions. As of yet, there are no clear methods of establishing critical conditions, especially in terms of the probability of occurrence. The analyst must use considerable judgement in selecting critical conditions for the particular system. Once loads and either critical conditions or estimated future conditions are specified, the calibrated model can be used to predict the water quality response. The investigation may involve study of extreme hydrological, meteorological, or hydrographic events that affect mixing; waste loadings from point and non-point sources; and changes in benthic demands.

Simplified Illustrative Examples

This section presents illustrative examples of estuarine modeling using both simple screening procedures and the water quality model WASP4. The screening procedures are based upon simple analytical equations and the more detailed guidance provided in "Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants - Part 2." WASP4 examples demonstrate model based estuarine WLA application.

WASP4 is a general multi-dimensional compartment model supported and available through the U.S. EPA Center for Exposure Assessment Modeling.

The examples provided consider eight water quality concerns in three basic types of estuaries. A one dimensional estuary is analyzed by screening methods for conservative and nonconservative toxicants and chlorine residual. Bacteria and DO depletion are simulated. Nutrient enrichment, phytoplankton production, and DO depletion in a vertically stratified estuary are simulated. Finally, ammonia toxicity and a toxicant in a wide, laterally variant estuary are simulated.

The screening procedures can be applied using calculator or spreadsheet. While they may not be suitable as the sole justification for a WLA, they can be valuable for initial problem assessment. Three screening methods are presented for estimating estuarine water quality impacts: analytical equations for an idealized estuary, the fraction of freshwater method, and the modified tidal prism method. These example procedures are only applicable to steady state, one-dimensional estuary problems.

Deterministic water quality modeling of estuarine systems can be divided into two separate tasks: description of hydrodynamics, and description of water quality. The WASP4 model was designed to simulate water quality processes, but requires hydrodynamic information as input. Hydrodynamic data may be directly specified in an input dataset, or may be read from the output of a separate hydrodynamic model. The examples here illustrate tidal-averaged modeling with user-specified hydrodynamics. Both the eutrophication and toxicant programs are described and used.

For the six examples using WASP4, background information is provided, the required input data are summarized, selected model results are shown, and certain WLA issues are briefly described.

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 allocation (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:

This part, "Part 1: Estuaries and Waste Load Allocation Models," provides technical information and policy guidance for the preparation of estuarine waste load allocations. It summarizes the important water quality problems, estuarine characteristics and processes affecting those problems, and the simulation models available for addressing these problems. The second part 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. The third part summarizes initial dilution and mixing zone processes, available models, and their application in waste load allocation. Finally, the fourth part summarizes several historical case studies, with critical reviews by noted experts.

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 Estuarine Waste Load Allocation Modeling

4. Monitoring Protocols for Calibration and Validation of Estuarine Waste Load Allocation Models

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4.1. General Considerations

This section addresses data needs for the calibration and validation of estuarine waste load allocation models. The type and amount of data will depend on: (1) the study objectives, (2) system characteristics, (3) data presently available, (4) modeling approach selected, (5) the degree of confidence required for the modeling results, and (6) project resources. Each of these factors should be considered in the planning stage of the monitoring effort in order to formulate fundamental questions that can be used in sample design.

Quantitative estimates should be made, wherever possible, of the gains or losses in model accuracy and precision due to different monitoring plans or modeled processes in order to provide a rational aid for making decisions governing the monitoring plan. For example, if study objectives require that boundary loads must be sampled with 95 percent confidence, then there are established quantitative methods available to estimate the sampling effort required (e.g. Cochran 1977, Whitfield 1982). The feasibility of study objectives can then be evaluated in terms of available resources and other study requirements.

Planning monitoring studies should be a collaborative effort of participants involved in budgeting, field collection, analysis and processing of data, quality assurance, data management and modeling activities. Collaboration insures that fundamental design questions are properly stated so that the available resources are used in the most efficient manner possible and that all critical data for modeling are collected. The use of monitoring and modeling in an iterative fashion, wherever possible, is often the most efficient means of insuring that critical data are identified and collected.

4.1.1. Study Objectives

The study objectives will often determine the degree of effort required for the monitoring study. The objectives should be clearly stated and well known prior to the planning of any monitoring study. Obviously, the purpose of such a study will be the allocation of waste loads for the water quality constituent of interest. However, the effort expended and the acceptable uncertainty in study results will depend largely upon the study objectives. For example, the monitoring program must be of much higher resolution if the main objective is to define hourly variations as compared to one where the objective is to determine the mean or overall effect of a waste load on an estuary. Until all objectives are defined it will be difficult to establish the basic criteria for a monitoring study.

4.1.2. System Characteristics

Each estuary is unique, and the scope of the monitoring study should be related to the problems and characteristics of that particular system. The kind of data required is determined by the characteristics of the system, the dominant processes controlling the constituent, and the time and space scales of interest. The same factors that control selection of modeled processes and resolution will be integral in determination of the monitoring required. A model can only describe the system, and that description can be no better than the data which determines how it is applied, drives it, and is used to evaluate its predictions. The particular advantages of models are that they can be used to interpolate between known events and extrapolate or project to conditions for which, for whatever reason, data are not available.

4.1.3. Data Availability

Some data have to be available in order to make initial judgments as to the location and frequency of samples as well as to make decisions concerning the selection and application of the waste load allocation model. Where data are not available for the constituents of interest then it may be necessary to use some alternative or surrogate parameters for these initial judgments. For example, suspended solids may be used in some situations as a surrogate for strongly sorbed constituents. Reconnaissance or preliminary surveys may be required to provide a sufficient data base for planning where only limited data are available.

4.1.4. *Model Selection*

A preliminary modeling approach should be selected prior to the monitoring study based on historical data and reconnaissance or preliminary surveys. Ideally, preliminary model applications should be conducted to assess the available data and provide guidance on monitoring requirements. Critical examination of the models input data requirements and studies of its sensitivity to parameters and processes should aid in the development of monitoring strategies. Several iterative cycles of data collection and model application serve to optimize both monitoring and modeling efforts.

4.1.5. *Confidence*

To a large degree the quantity and quality of the data determine the confidence that can be placed on the model application. Without data, it is impossible to determine the uncertainty associated with model predictions. Uncertainties in the determination or estimation of driving forces for the model (e.g. loadings, wind) will be propagated in model predictions. The greater the uncertainty (spatial, temporal or analytical) associated with data used in model forcing functions, estimation of model parameters, or evaluation of model predictions, the greater the resulting uncertainty associated with those predictions. One fundamental issue that may impact monitoring studies is the acceptable degree of uncertainty in both data and model projections.

4.1.6. *Resources*

All waste load allocation studies will be limited to some degree by budgetary, manpower, laboratory, or other constraints. The limited resources will probably require that the number of stations and/or the frequency of sampling be restricted. The planning of the data collection program should involve analysis of various sampling strategies and their associated cost. The planning should include factors such as the logistics and scheduling of crews, boats, equipment, meals, sample storage and preservation, acceptable holding times, laboratory preparation, communications, backup for equipment failure, quality assurance and other resource intensive factors that affect the successful completion of data collection efforts. An objective of any such planning study then is to maximize the information obtained for the given project resources. For major studies, the time and effort for this planning effort should be carefully considered and included in project plans.

4.2. Types of Data

The data collected in support of an estuarine waste load allocation study will be used to (1) determine the type of model application required, (2) drive the model, (3) provide a basis for assigning rate coefficients and critical model input parameters, and (4) determine if the model is adequately describing the system. The methods for using this data in the calibration and validation of models is the topic of Section 5.0. The general types of data required are described below.

4.2.1. *Reconnaissance and/or Historical Data*

Data are required initially to define the problem and determine the type of model solution required. For example, determination of appropriate model resolution must be based on available data. Historical data should always be surveyed. Historical data should be verified to insure that sampling techniques and laboratory analysis procedures have not changed which might make the historical data unsuitable for comparative purposes. Where historical data are not available it may be necessary to perform reconnaissance studies to obtain sufficient data for planning. A reconnaissance study as defined here is a survey of the site to obtain sufficient data to make preliminary judgments. Additional reconnaissance studies may be required particularly in areas where the greatest uncertainties exist. The reconnaissance level data is important not only in defining the more intensive monitoring effort but also in determining the modeling approach and resolution.

4.2.2. *Boundary Conditions*

Boundary condition data are <u>external</u> to the model domain and are driving forces for model simulations. For example, atmospheric temperature, solar radiation and wind speeds are not modeled but are specified to the model as boundary conditions and drive modeled processes such as mixing, heat transfer, algal growth, reaeration, photolysis, volatilization, etc. Nonpoint and point source loadings as well as inflow water volumes are model boundary input. The boundaries at the upstream end of the estuary and the open boundary at the ocean provide major driving forces for change. Models do not make predictions for the boundary conditions but are affected by them.

4.2.3. *Initial Conditions*

Generally, initial conditions are not required for internal flows or velocities. However, for water quality constituents initial conditions are required where the period of interest in simulations is less than the time required for these initial conditions to be "flushed out". For example, if the model is to be run to steady-state, then by definition initial conditions are not required. However, if simulations are to be conducted over "short" (in relation to the flushing time) periods of time, then initial conditions may be critical. Where changes are small, the initial conditions may dominant projections making it difficult to determine sources of error, such as in modeling approaches.

4.2.4. Calibration

Most estuarine hydrodynamic and water quality models are general in that they can be applied to a variety of sites and situations. However, the values of model parameters may be selected on a site specific basis, within some acceptable range. The process of adjusting model parameters to fit site specific information is known as model calibration, and requires that sufficient data be available for parameter estimation. The data base should include not only information on concentrations for the parameters of interest but on processes affecting those concentrations, such as sediment oxygen demand, settling and resuspension velocities, etc. While resources often limit the extent of the calibration data, more than one set describing a range of conditions is desirable.

4.2.5. Validation/Evaluation

It is always wise to test the calibration with one or more independent data sets in order to insure (or validate) that the model accurately describes the system. Validation conditions should be sufficiently different from calibration conditions to test model assumptions without violating them (where the assumptions are considered reasonable). For example, if the rate of sediment oxygen demand is assumed not to change (i.e. is specified as a zero order rate), then the model obviously would not predict well under situations where the sediment oxygen demand was drastically different due to some event. A second example is that an application assuming constant morphometry could not be expected to perform well after flood events, dredging, or construction resulted in variations in that morphometry. Discussions of the procedures for model validation/evaluation are provided in Chapra and Reckhow (1983) and Thomann and Mueller (1987).

4.2.6. Post Audit Data

One type of data that is often ignored is post-audit data. Generally, models will be calibrated and validated and then applied to make some projection about conditions, such as the effects of waste loads. The projections are often then used as an aid in making regulatory decision. This is often the end of most modeling and monitoring studies. There are relatively few cases where studies are conducted after the implementation of those decisions to determine if the model projections were accurate and management decisions appropriate. However, without this type of data the overall success or failure of modeling studies often can not be accurately assessed.

4.3. Frequency Of Collection

The frequency of data collection depends on all the factors mentioned in part 4.1. However, two general types of studies can be defined - those used to identify short term variations in water quality and those used to estimate trends or mean values.

4.3.1. Intensive Surveys

Intensive surveys are intended to identify intra-tidal variations or variations that may occur due to a particular event in order to make short-term forecasts. Intensive surveys should encompass at least two full tidal cycles of approximately 25 hours duration (Brown and Ecker 1978). Intensive surveys should usually be conducted regardless of the type of modeling study being conducted.

Wherever possible, all stations and depths should be sampled synoptically. For estuaries that are stationary wave systems (high water slack occurs nearly simultaneously everywhere), this goal may be difficult to achieve due to the logistics and manpower required. Synoptic sampling schemes are constrained by distance between stations, resources in terms of manpower and equipment, and other factors which may limit their applicability. Where it is not possible to sample synoptically, careful attention should be given to the time of collection. For some estuaries, where movement of the tidal wave is progressive up the channel, sampling the estuary at the same stage of the tide may be possible by moving upstream with the tide to obtain a synoptic picture of the water quality variations at a fixed tide stage, that is a lagrangian type of sampling scheme (Thomann and Mueller 1987). Sampling should not be conducted during unusual climatic conditions in order to insure that the data is representative of normal low flow, tidal cycle and ambient conditions.

Boundary conditions must be measured concurrently with monitoring of the estuary. In addition, a record of waste loads during the week prior to the survey may be critical. It is necessary to identify all of the waste discharging facilities prior to the survey so that all waste discharged can be characterized. Estimates of nonpoint loads are also required.

Where project resources limit the number of samples, an alternative may be to temporally integrate the samples during collection or prior to analysis. This will, however, not provide information on the variability associated with those measurements.

4.3.2. Trend Monitoring

Trend monitoring is conducted to establish seasonal and long term trends in water quality. Intensive data is not sufficient to calibrate and validate a model which will be used to make long-term projections, due to differences in the time scales of processes affecting those projections. Trend sampling may take place on a bi-weekly or monthly basis. Stations should be sampled at a consistent phase of the tide and time of day to minimize tidal and diurnal influences on water quality variations (Ambrose 1983). Diurnal variations must still be considered, however, tidal effects may be less important in wind dominated estuarine systems. Care should be exercised to sample during representative conditions and not during unusual climatic events in order to allow comparison between sampling times. Some stations may be selected for more detailed evaluation. Intensive surveys, spaced over the period of monitoring, should also be considered where the trend monitoring will be used to track changes in parameters between intensive surveys (Brown and Ecker 1978).

Boundary data should generally be measured at a greater frequency than estuarine stations used for monitoring trends. Boundary conditions are critical in that they will drive the model used for waste load allocation. The rate at which the boundary conditions are expected to change will indicate the time scale required for boundary sampling. Tiered or stratified sampling programs may be required which include different sampling strategies, such as between low and high flow periods. The more intensive boundary data will provide an estimate of the mean driving forces for the model as well as their associated variability.

The type of boundary data required is discussed in the next section. Generally, data on flows, meteorology and water level variations may be available more frequently than necessary for water quality parameters. The variability associated with the observations can be used to estimate the sampling effort required for a given acceptable degree of confidence using well established methods (see Cochran 1977, Gilbert 1987, Elliott 1977 or others). For example, where the mean and standard error of a constituent have been estimated from reconnaissance studies and the error is simply inversely proportional to the sample size, the sample size required to obtain an acceptable error rate can easily be determined. The frequency required for water quality parameters for tributaries may be estimated using ratio and regression methods to determine the uncertainty associated with loading estimates for various sampling designs (see for example Cochran 1977; Dolan, Yui and Geist 1981; Heidtke, DePinto and Young 1986).

4.4. Spatial Coverage

An intensive spatial coverage of the estuary for some indicator or surrogate water quality parameter, such as salinity or turbidity, is generally needed in order to estimate spatial variability, as well as determine the model type and segmentation required.

Generally, the spatial grid for an estuarine model should extend from above the fall line, or zone of tidal influence, to the open boundary of the estuary. The last USGS gauging station is often a good upper boundary since they are typically placed outside of the region of tidal influence. In some cases the ocean boundary will extend beyond the estuary into the ocean to insure a representative boundary condition or to allow use of tidal gauge information collected at some point away from the estuary.

Where simple waste load allocation studies are planned on a portion of an estuary, and it is unrealistic to model the entire estuary, then the spatial grid may be delimited by some natural change in depth or width, such as a restriction in the channel or regions where the velocity and water quality gradients are small. The spatial grid must encompass the discharges of interest in all cases.

Sampling stations should generally be located along the length of the estuary within the region of the model grid, with stations in the main channel and along the channel margins and subtidal flats for the intensive surveys. Lateral and longitudinal data should be collected, including all major embayments. The spatial coverage required is governed by the gradients in velocities and water quality constituents. Where no gradients exist, then a single sample is sufficient. Some caution should be exercised in the selection of the indicator parameter for this decision. For example, strong vertical dissolved oxygen gradients may occur in the absence of velocity, thermal or salinity gradients. Two areas where cross-channel transects are generally required are the upper and lower boundaries of the system. Additional sampling stations may also be selected so that poorly mixed discharges can be adequately detected and accounted for.

The spatial coverage should consider the type of model network to be used. For model networks with few, large segments, several stations (e.g. 3-6) should be located in each model segment in order to estimate spatial variability. For detailed models with many segments it may not be possible to determine the parameters for each segment. For initial conditions and model evaluation, sufficient samples should be collected to estimate missing data by interpolation.

Where resources are limited, one possible monitoring strategy is to spatially integrate samples, such as over depth or width depending on the modeling approach used. Careful consideration will need to be given to the integration scheme for this type of monitoring. For example, a flow weighted integration scheme would require some *a priori* knowledge of the fraction of the total flows associated with all sampling stations.

4.5. Model Data Requirements

4.5.1. Estuary Bathymetry

Data are always required to determine model morphometry. Morphometry affects the characterization of the estuary and the type of modeling approach required. Estuarine depth controls propagation of the tidal wave. Shallow channels and sills increase vertical mixing while deep channels are more likely to be stratified with greater upstream intrusion. Deep fjords with shallow sills usually have little circulation and flushing in bottom waters. The length of the estuary determines the type of tidal wave, phase between current velocities and tidal heights. The width effects velocities (narrow constrictions increase vertical mixing and narrow inlets restrict tidal action). Wind-induced circulation is transient and interacts with channel geometry to produce various circulation patterns and affects vertical mixing and sediment transport.

Bathymetric data are available for most estuaries from U.S. Coastal and Geodetic Navigation Charts and Boat Sheets or from sounding studies conducted by the U.S. Army Corps of Engineers. The National Oceanographic Survey can provide data on computer tapes. The charts tend to slightly underestimate depths in navigation channels to allow for siltation. Alternatively, a vessel traveling along established transects can measure depth profiles with a high frequency fathometer connected to a continuous strip-chart recorder. Depths must be corrected to mean tide level at the time of measurement (Kuo et al. 1979). Slopes of the water surface should also be considered in data reduction. Fathometer frequencies used in measuring bottom depths should be between 15 and 210 KHz (wavelengths between 85 and 6 mm). Short wavelengths are most useful for measuring soft, muddy bottoms, while long wavelengths are used with a hard, firm bottom (Ambrose 1983).

For certain estuaries, such as many of those along the Gulf of Mexico, the affects of tidal marshes can dramatically effect estuarine circulation and water quality. These are generally some of the more difficult systems to model. An initial decision may be whether to measure flows and quality and provide information to the model as boundary conditions or to attempt to model them. Where modeling is required then the corresponding bathymetry data must be collected.

Table 4-1. Estuarine Transport Data

Morphometry Data:	Channel Geometry, "roughness" or bottom type
Hydrodynamic Data:	Water surface elevations Velocity and direction Incoming flow Point and distributed flows
Meteorological Data:	Solar radiation Air temperature Precipitation Wind speed and direction Wave height, period and direction Relative humidity Cloud cover
Water Quality Data:	Salinity Water temperatures Suspended sediments Dye studies

4.5.2. Transport

Either description or prediction of transport is essential to all waste load allocation studies. All mechanistic waste load allocation models are based on mass balance principles, and both concentrations and flows are required to compute mass rates of change. For example, a loading to the system is expressed in units of mass/time, not concentration. Essential physical data required for prediction or description of transport are listed in Table 4-1.

The type of data used to quantify transport depends upon the model application and the characteristics of the system (i.e. well mixed, partially mixed or highly stratified estuary). Estuarine geometry, river flow and tidal range, and salinity distribution (internal, inflow and boundary concentrations representative of conditions being analyzed) may be sufficient for applications involving fraction of freshwater, modified tidal prism methods, or Pritchard's methods (as described in Mills et al. 1985). Models such as QUAL2E (Brown and Barnwell 1987) can also be applied to estuaries using this data where vertical resolution is not a concern, using net flows and a tidal dispersion coefficient.

For complex estuaries, time varying flows, depths, and cross sections will make estimation of flows and dispersion from field data difficult. Then the flows have to be measured, estimated from dye studies, estimated by trial and error methods, or obtained from hydrodynamic studies. However these parameters are determined they must adequately reflect the flushing characteristics of the system. Data requirements for flow measurement and hydrodynamic modeling are discussed below.

4.5.2.1. Flow Measurement

Flow measurements can be used directly in waste load allocation models or be used to aid in the calibration and validation of hydrodynamic models, as discussed below. Tidal current is determined by placing a network of current meters at selected stations and depths throughout the estuary and measuring velocities over time. A tidal velocity curve can then be constructed. The data measured at different points can be integrated over space (i.e. laterally or vertically) and/or time depending on the needs of the water quality model. Data from the flow measurements should be evaluated when incorporated into models to insure that continuity is maintained and that constituents are properly transported.

Freshwater inflow measurements are often available for major tributaries from USGS records or from state agencies. Daily records are normally available and hourly or 15 minute records can often be obtained. The frequency at which data are required must be assessed in the context of how rapidly flows are changing. Generally, hourly and often daily data are sufficient. Flows must be estimated for ungauged tributaries, and where the influence of ungauged tributaries is appreciable, a flow monitoring program initiated. Groundwater inflows or flows from direct runoff may be estimated from flow gauges available in the fluvial portion of most large drainage basins. Inflows from point source dischargers, including municipal and industrial sources and combined sewer overflows are essential input to any model.

4.5.2.2. Dye Studies

Dye and time of travel studies are often one of the better sources of data for estimating dispersion coefficients, computing transport or for calibration and confirmation data for hydrodynamic models. Dye studies can be conducted with injections toward the mouth of the estuary or in areas where there is the greatest uncertainty in model predictions. For example, dye studies can be used to estimate mixing in the freshwater portion of a tidal river where no salinity gradients occur.

The type of dye study conducted varies with the study objectives. Studies may involve continuous or slug releases of the tracer dye. Continuous discharges are particularly useful in estimating steady-state dilution levels while slug studies are often useful for estimating dispersion coefficients or for calibrating and testing hydrodynamic models.

Continuous tracer studies generally release dye over one or more tidal cycles or discharge periods, which is then monitored within the estuary at selected locations over a series of tidal cycles. Monitoring of continuous dye releases may be continuous or concentrate on initial dilution and successive slack tides to obtain wastewater dilution levels for initial dilution, high and low slack tides or tidally averaged conditions. The superposition principal developed by the U.S. Geological Survey (Yotsakura and Kilpatric 1973) can be used to develop wastewater dilutions.

A slug of dye may be injected into the system and then the dye cloud is tracked over several tidal cycles. The spread of the dye and/or attenuation of the dye peak will aid in estimation dispersion coefficients, and the movement of the dye centroid will give an estimate of net flows. The computations usually involve solving the transport equation in some form where the known quantities are geometry and time varying dye concentrations and the unknowns are advection and dispersion. Diachishin (1963) provides guidance on estimating longitudinal, lateral and vertical dispersion coefficients from dye studies. Fischer (1968) described methods for predicting dispersion in applications to the lower Green and Duwamish Rivers, estuaries of Puget Sound. Carter and Okubo (1972) described a technique to estimate a longitudinal dispersion coefficient from peak dye concentrations and describe the slug release method used in Chesapeake Bay. Thomann and Meuller (1987) provided an example of computing tidal dispersion coefficients from a slug release of dye into the Wicomico River, an estuary of Chesapeake Bay. Some caution should be exercised in that dyes injected at a point will have different travel times from those mixed over the modeled dimensions. For example, for a one-dimensional (longitudinal) model it may be preferable to distribute the dye as a vertically mixed band across the estuary.

A variety of dye types have been used in the past, and a comparison of tracer dyes was provided by Wilson (1968) as well as an overview of fluorometric principals. The most common dye presently in use is Rhodamine WT. The U.S. Geological Survey (Hubbard et al. 1982) provides information on planning dye studies which has applicability to estuaries. Generally boat mounted continuous flow fluorometers can be best used to locate and track a dye cloud or to obtain dye concentrations at discrete stations. Some consideration should be given to the toxicity of the dye as well as to its degradation by chlorine in studies of treatment facilities or its absorption onto particulates and macrophytes. Rhodamine WT is also slightly more dense than water and may require adjustment to obtain neutral buoyancy. The background florescence should be determined to aid in determining quantities of dye to be released and subtracted from field measurements. Care should also be exercised to schedule dye studies to avoid non-representative meteorological conditions. Some of the considerations for planning and conducting dye studies in estuaries were discussed by Story et al. (1974).

4.5.2.3. Hydrodynamic Models

Hydrodynamic models may be used to generate flow fields for waste load allocation models. Major processes impacting transport in estuaries incorporated in hydrodynamic models include river flow, tidal action, fresh and salt water mixing, salinity gradients and stratification, wind stress, coriolis force, channel geometry and bottom friction. Data required to drive the hydrodynamic models includes initial and boundary conditions as well as calibration and validation data.

Generally, unknowns solved for in hydrodynamic models include velocities and water surface elevations. However, most hydrodynamic models applicable to estuaries include forces due to changes in density and, as such, include transport of salinity and possibly temperature to be coupled with the hydrodynamic equations at the intra-tidal time scale. The accurate prediction of water surface elevations or velocities is not sufficient to test the model application for waste load allocation purposes, but the models must also accurately transport materials as well. Therefore, data requirements as discussed below will include constituents such as salinity, temperature, and other tracers which can be used to evaluate hydrodynamic predictions. An intensive data sampling program which includes concurrent water surface elevation, velocity and dye/dispersion studies or salinity profiles provides the best assessment of the hydrodynamic model application.

A. Initial conditions

Initial conditions are generally not required for flows in hydrodynamic models. Generally, velocity fields are set up within relatively few model time steps. Initial conditions are required for materials such as tracers, salinity or temperature used to validate transport predictions. An exception is where the initial conditions are rapidly flushed, or the flushing period is short in comparison to the simulation period. For rapid flushing it is often reasonable to run the model to a steady-state using the initial boundary conditions and use the results of steady-state simulations as the initial conditions for subsequent simulations. Where initial conditions are required, data will generally not be available for all model segments, due to the fine spatial resolution required in hydrodynamic models. Where data are not available it may be possible to estimate missing data by interpolation.

B. Boundary conditions

Hydrodynamic boundary conditions consist of flows or heads. Head refers to the elevation of the water surface above some datum. Generally, flow information is provided for tributary and point sources and water surface elevations provided for the open (ocean) boundary(ies). Salinity, and often temperature, conditions may be required at the boundaries in order to estimate density effects on circulation (baroclinic effects).

Water surface elevation information is often available for major estuaries from tide gauge records such as the Coast and Geodetic Survey Tide Tables published annually by NOAA. These records may be processed into tidal constituents. Records are often available for time periods of 15 minutes which is usually sufficient for model application. These tide tables do not include the day-to-day variations in sea level caused by changes in winds or barometric conditions, nor do they account for unusual changes in freshwater conditions. All of these conditions will cause the tide to be higher or lower than predicted in the tables. The data can however be used to determine if the data collected in the sampling period is "typical (Brown and Ecker 1978). Where possible, water surface elevation gauges should be placed at the model boundaries as part of the monitoring program.

Meteorological data, including precipitation, wind speed and direction are required to compute surface shear, vertical mixing and pressure gradients. Meteorological data are often available for nearby National Weather Service stations from the National Climatic Center in Asheville, North Carolina. However, the class of the stations should be identified to determine if all the required data are available. If the estuary is large or nearby stations are unavailable then either the use of several stations or field monitoring of meteorological conditions may be required. If temperature is to be simulated, as part of the hydrodynamic model evaluation or for water quality modeling purposes, then data on air temperature, cloud cover, humidity and precipitation must be available. Evaporation data should also be evaluated. Solar radiation and the effects of coriolis forces can be computed from the location of the estuary and time of the year.

Boundary data are required for water quality constituents used to calibrate and validate transport predictions, such as salinity and temperature. The frequency of data collection for tributaries and point sources was discussed previously (see section 4.3). The sampling stations for tributaries should generally be above the fall line, or region of tidal influence. The open, or ocean boundary, is generally specified as either constant or time-varying conditions which are not impacted by interactions with the estuary. In some cases this may require that the model and its boundary be extended into the ocean to a point where this assumption is valid or to where data are available. The station(s) used for open boundary should be determined with careful consideration of the model application.

C. Calibration and validation data

Calibration and validation of hydrodynamic predictions can consist of comparison of model predictions to measured velocities or water surface elevations. Measurements of water surface elevations and current velocities at critical sampling locations should be included as part of the monitoring effort. The placement of the current meters should be based, at least in part, by the model application. For example, a single continuous monitor placed at the edge of a channel would provide little usable information for a laterally averaged model, where laterally averaged velocities at a given depth are required for comparison.

As stated previously, the accurate predictions of water surface elevations and velocities are not sufficient for testing the application of a hydrodynamic model where those velocities will be used to determine constituent transport. Additional testing must be conducted to determine if the transport is reasonable and if known water quality gradients can be maintained. For example, the effects of an overestimation of vertical velocities, which are often too small to be accurately measured in the field, may only become apparent when the transport model is unable to maintain known vertical profiles.

The calibration of the hydrodynamic model may require an iterative effort in conjunction with the application of the water quality models for the constituents of interest (i.e. dissolved oxygen). However, initial calibration is usually conducted against materials such as conservative tracers, salinity, or temperature. Salinity, temperature and suspended solids concentrations will impact density which will in turn affect computed velocity distributions. The transport of at least salinity and possibly temperature and suspended solids should generally be directly linked to hydrodynamic predictions for estuaries (i.e. their effects are considered in density terms).

4.5.3. Water Quality

The water quality data required, beyond that needed to quantify transport as described above, will vary depending on how the variables will be used and their anticipated impacts on the waste load allocation analysis. In addition, the water quality data required will vary depending on the anticipated response time of the system to changes in the value of the variable. For example, processes that vary over long time scales, in relation to the period of modeling, are often assumed to have a constant effect over the period of simulation (treated as zeroth order processes). Sediment oxygen demand and sediment release rates are often treated in this way.

Data requirements will vary if the waste load allocation is intended for dissolved oxygen, eutrophication or toxics. Variables critical for an analysis of toxicity, such as pH for ammonia and metals, may not be required if the parameter of interest is DO. If the waste load is not expected to impact particular variables, such as pH, then it may be sufficient to use available data to determine their effects. If however, data are not available for conditions of interest, or if the variable is expected to change, either directly or indirectly, in response to the loading, then modeling may be required as well as collection of additional supporting data.

Table 4-2 provides an overview of some commonly measured water quality variables, their problem contexts, and an indication of the processes they impact. Some variables, such as dissolved oxygen (DO) are suggested for all studies. DO can provide general information about the estuaries capacity to assimilate polluting materials and support aquatic life (MacDonald and Weisman 1977). The specific type of data for a particular application will vary depending on the factors listed in section 4.1. Concentrations for all pertinent water quality variables should be provided at the model boundaries, providing the driving forces for model predictions, as well as at stations within the model system to provide a basis for estimating model parameters and evaluating model predictions.

Measurements of processes impacting water quality may be required in addition to concentration measurements. For example, strongly sorbed contaminants are strongly affected by sediment interactions, including resuspension, settling, and sedimentation. Some independent measurement of these processes may be required to reduce model uncertainty. Modeled processes for a variety of water quality constituents and the data requirements for those process descriptions are provided by Ambrose et al. (1988a,b).

4.6. Quality Assurance

A rigorous, well documented, quality assurance (QA) plan should be an integral part of any waste load allocation program. The QA plan should include descriptions of sampling collection, preservation, handling, analysis, analytical detection limits, and data management. The implemented plan should provide a well documented record of all stages of the project, extending from sampling and transferring custody of samples, to modeling. The development of the plan should be completed prior to the initiation of any monitoring activities and a quality assurance coordinator assigned to implement and coordinate QA activities. There are a variety of documents which describe procedures for quality assurance, and a complete description of a quality assurance plan is beyond the scope of this report. Additional information is provided in:

- Guidelines and Specifications for Preparing Quality Assurance Project Plans. USEPA Office of Research and Development, Municipal Environmental Research Laboratory. 1980.
- Standard Methods for the Examination of Water and Wastewater, 15th Edition. American Public Health Association. 1980.
- Methods for the Chemical Analysis of Water and Wastes. EPA-600/4-79-020. USEPA Environmental Support Laboratory. 1979.

Table 4-2. Water Quality Variables

Constituent	Problem Context	Effects
Salinity or Conductivity	All	Transport, dissolved oxygen
Temperature	All	Transport, kinetics, dissolved oxygen, toxicity
Suspended Solids	All	Transport, light extinction, sorption
UV Light	Eutrophication, Toxics	Heat, algal growth, photolysis
Light Extinction	Eutrophication, Toxics	Heat, algal growth, photolysis
Dissolved Oxygen	All	Indicator, toxicity, sediment release
BOD-5	DO	Dissolved Oxygen
Long Term CBOD	DO	Dissolved Oxygen
Carbon Dioxide	Toxics, Eutrophication	
NBOD	DO	Dissolved Oxygen
Bottom Demand	Eutrophication DO	Dissolved Oxygen, nutrient release
Total phosphorus	Eutrophication DO	Algae
Soluble reactive phosphorus	Eutrophication DO	Algae
Total kjeldahl nitrogen	Eutrophication DO	Dissolved oxygen, algae
Ammonia-nitrogen	Eutrophication DO, Toxicity	Dissolved oxygen, toxicity, algae
Nitrate-nitrogen	Eutrophication DO	Dissolved oxygen, algae
Nitrite-nitrogen	Eutrophication DO	Dissolved oxygen, algae
Dissolved available silica	Eutrophication DO	Algae
Chlorophyll-a and Phaeophyton	Eutrophication DO	Algal indicator
Phytoplankton (major groups)	Eutrophication DO	Dissolved oxygen, nutrient cycles, pH
Alkalinity	Toxics	pH, carbonate species, metals
Total inorganic carbon	Toxics	pH, carbonate species, metals
pH	Toxics	Speciation, ionization, toxicity
Contaminant (dissolved particulate, total)	Toxics	Allocation
Dissolved organic carbon	Toxics	Sorption, activity
Total organic carbon	Toxics	Sorption, activity
Porosity	Sediments	Pore water movement, toxicity
Grain size	Sediments	Settling, sorption, sediments
Percent solids	Sediments	Sorption, sediments
Eh	Toxics, DO	Indicator, speciation
Biomass	Toxics	Biouptake
Meteorologic Data wind, temperature, etc.	All	Gas transfer, reaction rates
Toxicity (cereodaphnia toxic units, etc.)	Toxicity	Toxicity
Coliform Bacteria (Fecal, Total, Streptococci)	Human Health	Human Health

- Handbook for Analytical Quality Control in Water and Wastewater Laboratories. EPA-600/4-79-019. USEPA Environmental Support Laboratory. 1979.

Discussion is provided below of some suggested elements of a QA plan.

4.6.1. Data Collection

All stations for data collection should be well described and documented in order to insure that they are reestablished during subsequent sampling periods. Stations can be established using an easily determined distance from some permanent structure or landmark. However, care should be exercised to insure that the stations are not located near some structure which would make them unrepresentative. For example, velocity measurements should not be made immediately downstream of a bridge or piling no matter how convenient it may be. Stations can be relocated using electronic positioning equipment such as range instruments, radar or Loran if they are sufficiently accurate to allow relocation within an acceptable distance. Methods should be established for maintaining positions at stations during sampling. Records of arrival and departure times for each site as well as surface observations should be made during each sampling period.

Instruments for electronic *in situ* determination of water quality parameters should be calibrated at least before and after each sampling trip. For example, samples should be collected for salinity to verify field measurements and samples fixed in the field for dissolved oxygen to verify dissolved oxygen probes.

All field collection equipment should be listed and prepared before each sampling trip, insuring that all collection containers are clean and proper log forms and labeling equipment available. Different containers should be available for metals, nutrients, organics, dissolved oxygen, etc. due to their cleaning and preservation requirements. The QA plan should contain a detailed description of techniques for samples requiring special handling, such as toxics and anaerobic samples.

An established sequence of collection should be developed and maintained throughout the monitoring effort, insuring that new personnel are trained in the proper methods and sequence of data collection. All samples should be logged and sample log sheets should include station location, time, depth, results of *in situ* sampling, and container numbers for each type of sample. Datum should always be clearly specified (e.g. time of day standard, datum for water surface elevations).

All samples should be preserved on board, where the preservation technique will vary with the type of analysis required, but may involve icing, acidification, organic extraction, etc. The preservation techniques should be documented prior to implementation of the monitoring study. For some samples that do not preserve well it may be necessary to either conduct analyses on board or quickly transfer them to nearby on-shore facilities.

Additional samples should be collected to determine sampling variability and individual samples may be split prior to analysis to determine analytical variability. The number of replicate samples should be established as part of the planning for the monitoring effort. Field samples may also be spiked with a known amount of a standard prior to analysis. The identity of the spiked, split and duplicate samples should be kept on separate logs and the analyst should not be aware of their identity.

The samples should be transferred from the field to the laboratory in a timely manner. The field logs should be recorded and a laboratory log kept of the samples and their arrival. Custody sheets may be kept to further document the transferral of samples.

4.6.2. Data Analysis and Release

Samples should be transferred from the field to laboratory personnel, and the laboratory personnel should log samples into the laboratory, noting the time and date received, sample identities and other pertinent information from the field logs. The samples should be checked for proper preservation and transferred to proper storage facilities prior to analysis. The laboratory QA plan should include timelines indicating time limits for the analysis, descriptions of the analytical tests, sample preparation or extraction methods, detection limits, and methods for evaluating the quality of the analytical results. Methods should be included to describe handling of samples where their chemical matrix may cause analytical problems, such as toxicity for BOD samples, matrix problems for metals, or oils in organic analyses. Methods should be outlined describing archiving techniques for samples and analytical data.

An analytical log should be maintained for each type of analysis, providing information on the sample identity, analyst, date and time of analysis, and where applicable, information on standard curves, blanks or baseline information, peak heights or meter readings, dilutions or concentrating methods, and computed concentrations. Observations should be included on any noted interferences or conditions which could effect the analysis. Strip chart or electronically produced information on the analysis should be ar-

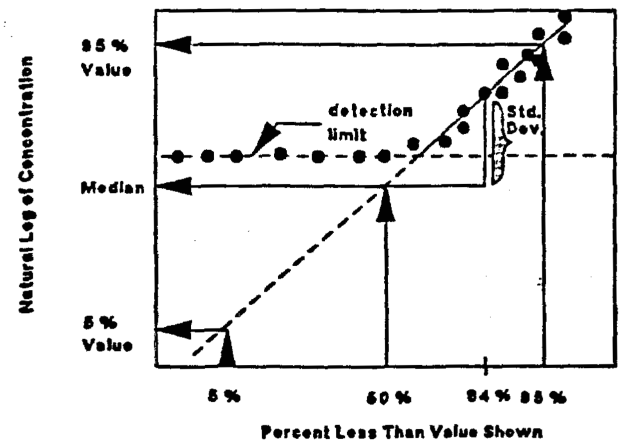

Figure 4-1. Illustration of use of log probability plot to estimate statistics for data including non-detects.

chived. Generally, the results of each analysis should be recorded on prepared forms for each sample containing information on the results of all analysis performed.

After completion of the analysis, the analytical results should be reviewed by the laboratory's quality assurance team to determine if the analytical results are acceptable. Methods should be established prior to implementation of the monitoring plan to check and identify the quality of the analytical results, insure the correct transferal of information and describe follow up procedures and corrective actions. The results should include indications of the analytical variability, as indicated by analysis of split samples, recovery of spikes, periodic laboratory audits and other methods. Wherever possible, questionable samples should be rerun. In some cases additional analysis may be included beyond the requirements of the modeling activities to insure the quality of the analytical results, such as to perform a dissolved solids or anion-cation balances where applicable.

Analytical results have little utility in mass balance calculations if those results are below, or clustered near, analytical detection limits. However, methods are available to estimate values where the statistical distribution of the samples are known or assumed. A method suggested by Thomann (R.V., pers. comm.) to analyze data including non-detects is to plot the data on log normal probability paper with a ranking of the data that includes those values below the detection limit (Figure 4-1). If the data are log normally distributed, the median and log standard deviation can be estimated from the plots and can then be used to estimate the mean using standard statistical transformations. This allows the estimation of statistics for data with values below the analytical detection limit. Where data are not sufficient to estimate statistics, based on assumptions regarding the statistical distribution of samples, it may be necessary to explore alternative analytical methods. Where more than one technique is used for a particular analysis care should be exercised to insure each sample is identified as to the type of analysis performed and its associated analytical variability.

The laboratory supervisors should maintain tracking records indicating the samples received, source, time of collection and their stage in the analytical process. This tracking record can be used to insure that samples are analyzed within preset time frames, aid in setting priorities, and inform data users of the status of the information they require. A common conflict occurs between laboratories wanting to prevent release of information until all possible checks are completed for all samples collected and data users who want any data they can obtain as quickly as possible. If preliminary or partial results are released, they should be properly identified indicating their status and updated when new information becomes available.

4.6.3. Data Management

QA plans should also extend to data management, insuring that data storage and retrieval mechanisms are established and that information on the identity and quality of the analytical results is maintained for each record. Care should be exercised to insure that the identity of the sample is preserved. Data should include time and location of collection, value, units, variability and information on significant figures and rounding procedures, and status as perhaps indicated by analytical codes. Checks should be established to insure that all data are recorded and that accurate transfer of information occurs between different media (such as between laboratory forms and data bases).

Modeling activities should be performed in a stepwise manner with testing at all stages in the application to insure that predictions are accurate and reasonable. The degree of model testing will be determined to some degree by the model's complexity and its previous history of testing and applications. However, a healthy skepticism is often the best method of avoiding errors and improper applications. All assumptions should be clearly stated and supported for independent review.

The QA for modeling activities should include, but not be limited to validation against independent data sets to insure that concentrations are accurately predicted. The QA activities should include calculations to insure that mass is properly conserved, numerical stability is maintained, and that model parameters are within reasonable ranges as reported in the literature. Analyses should be conducted of the confidence associated with the predicted results.

Wherever available, model testing should not be limited to comparisons with concentrations but model components should be compared to available data to insure that they are reasonable. For example, productivity data for a system could be computed for eutrophication models and compared to field data. A component, or mass balance, analysis will also provide information on the dominant factors affecting predictions (see Thomann and Meuller 1987).

A model application should be most accurate in estimating conditions that occur between those measured for calibration and validation, analogous to interpolation. However, model applications often require projection or extrapolation to conditions outside of the range of available data, such as to "pristine" conditions or to determine recovery times after a particular source has been eliminated. The variability associated with the projections can be determined to some degree by evaluation of the historical variability in forcing functions. However, testing of the model assumptions can often be determined only through comparisons with similar previous applications or with data collected after implementation of strategies based on those model projections. Wherever possible, such post-audit studies should be considered as part of the monitoring and modeling plans. The QA plan for modeling should also include methods to insure that, at a minimum, the input data used to drive the model in final calibration and validation simulations and copies of the computer codes and their users manuals used for prediction and manipulation are archived for later use. The archived files should contain a description of all of the files necessary to do the analysis and sufficient information to allow duplication of the reported results.

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5. Model Calibration, Validation, and Use

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5.1. Introduction And Terminology

This section describes procedures for selecting model parameters and coefficients that result in a calibrated model of the estuary of interest. Also described are procedures necessary to ensure that the calibrated model is validated for an appropriate range of conditions. Third, model testing procedures needed to calibrate and validate models are reviewed and assessed. Finally, guidance on how the calibrated model can be utilized in a waste load allocation to describe existing conditions and project the effects of reducing or increasing loads into the estuary, is provided.

Section 5.2 reviews a general procedure for calibrating models of the dissolved oxygen balance, of the nutrients that cause eutrophication problems, and of toxic chemicals and sediment. A comprehensive listing in a series of Supplements assists in defining the set of potential model coefficients and parameters that may be required to calibrate a model for waste load allocation. The Supplements are provided for each of the important coefficients and give specific guidance on how these parameters can be selected.

Section 5.3 briefly describes the validation procedure that is intended to estimate the uncertainty of the calibrated model and help establish that the model formulation chosen is at least useful over the limited range of conditions defined by the calibration and validation data sets. Section 5.4 reviews important statistical methods for testing the calibrated model. These methods are useful to aid in the various calibration phases and in the validation phase to measure how well model predictions and measurements of water quality agree.

Section 5.5 provides limited guidance on the utilization of a calibrated model for waste load allocation. Methods to determine causes of existing conditions and to project effects of changes in waste loads are discussed. Presently, methods to modify model coefficients such as sediment oxygen demand rates and deoxygenation rate coefficients are not well developed.

Model calibration is necessary because of the semi-empirical nature of present day (1989) water quality models. Although the waste load allocation models used in estuary studies are formulated from the mass balance and, in many cases, from conservation of momentum principles, most of the kinetic descriptions in the models that describe the change in water quality are empirically derived. These empirical derivations contain a number of coefficients and parameters that are usually determined by calibration using data collected in the estuary of interest. Occasionally, all important coefficients can be measured or estimated. In this case, the calibration procedure simplifies to a validation to confirm that the measurements of the inflows, the seaward conditions, and the conditions in the estuary are consistent according to the model formulation chosen to represent the water quality relationships. More often than not, it is not possible to directly measure all the necessary coefficients and parameters.

In general, coefficients must be chosen by what is in essence a trial and error procedure to calibrate a model. There is guidance on the appropriate range for coefficients but because each estuary is unique, there is always a chance that coefficients will be different from any other observed condition and fall outside the range. Because unique coefficients outside the normal ranges can also result if inappropriate model formulations are used, it becomes necessary to adopt, as much as possible, well accepted model formulations and to use standardized methods of testing the adequacy of calibration and validation. Also very important is the experience required to be able to determine when model formulations are not quite adequate. In this regard, it remains difficult to say how much experience is enough but this should not prevent the inexperienced from attempting this type of analysis. Many studies are straightforward enough so that extensive experience is not always mandatory.

If one accepts that calibration is basically a trial and error procedure, it can be quickly recognized that the methods involved should be as efficient as possible. To achieve some efficiency, there are two similar principles that should be applied. These are:

1. The universal caveat that the simplest model formulation should be used to solve the problem at hand, and

2. Principle of Parsimony.

The first caveat probably originated soon after the wide spread use of water quality models began in the 1960s (Schnelle et al. 1975). The use of simpler models remains a useful goal, but it should not be pursued zealously. For example, it should be kept in mind that the complete solution of the modeling problem may invölve simulation and prediction of effects on constituents that are unimportant during the calibration phase. The benthic flux of nutrients may become more important when point sources are cleaned up and may need to be included in any long term projection. Also, modelers should use codes with which they have the most experience and confidence in, as long as this does not complicate the analysis or avoid including important elements of the water quality processes. Finally, NCASI (1982) demonstrates that for stream water quality modeling, that overly simplistic models can be calibrated (due to the flexibility built into general purpose models) and unless rigorous validation procedures are followed, the errors involved will not be obvious. Since some estuarine conditions are quite similar to riverine conditions, these conclusions are also valid for estuarine modeling. Therefore, reasonably simple models should be used, but the effects of the approximations involved must be investigated.

The Principle of Parsimony (terminology suggested by Robert V. Thomann in review) is similar to the caveat that the simplest model should be employed but is more comprehensive in concept. Also included is the idea that model coefficients and parameters should be spatially and temporally uniform unless there is specific data or information demonstrating that the coefficients change. For example, it is very poor practice to vary coefficients from one model segment to the next unless there are well defined changes in the physical, chemical, or biological characteristics. When parameters are allowed to vary from one segment to the next to cause an exact match between predictions and measurements, the selected coefficients are contaminated with an accumulation of measurement errors from the field data and approximation error for the model formulations chosen. This assumes that water quality model equations are exact descriptions of the physical, chemical, and biological processes. This is never true for the currently available models (1989). Typically, this contamination causes rapid variation of coefficients from segment to segment when few data are available and the data are error prone. Values occasionally fall outside normal or typical ranges. In essence, this poor practice avoids the necessary use of engineering or scientific judgement in evaluating the limitations of the model chosen and in evaluating uncertainty in field data. It reduces the procedure to a grossly empirical curve fitting exercise. Since statistical curve fitting analysis has not been employed for the analysis of most water quality parameters of interest for several decades, this indicates that the model user is not sufficiently experienced in most cases to perform a waste load allocation.

The calibration procedure also involves investigation of the measurements that define the boundary conditions. In many cases, it is never clear that all loads can be adequately measured until the model is calibrated. Strictly speaking, it is not correct to use a calibration procedure to investigate measurements of loads and to define kinetic rates, parameters, and formulations. In general, this is a poor way to confirm that load measurements are adequate and when some loads are missed or over estimated, the optimum coefficients are error prone. When significant calibration errors occur, the calibrated model has very little predictive validity (i.e., the predictions are expected to be inaccurate) and the description of causes of water quality problems can be misleading.

In practice, however, there are no alternatives except to collect selected concentration data that can be used to indicate if loads are adequately measured. Other measurements of water quality concentration can be oriented to providing optimum calibration data to aid in the selection of accurate parameters. This practice requires some artful selection of parameters to be measured and of measurement locations and frequency. For example, dissolved solids and other conservative constituents should be simulated, especially those natural tracers occurring in point and non-point sources. Where undocumented sources are suspected, curtains of stations or upstream and downstream stations can be used to perform localized mass balances in portions of the estuary to indicate if any loads are not measured. (Here we use upstream and downstream to imply a localized mass balance in the riverine sections of the estuary.)

Other types of concentration measurements can be performed to better calibrate water quality kinetics. These measurements should be focused in areas some distance from suspected loads but where large water quality gradients are suspected. This may involve measurements away from shorelines and areas with contaminated sediments.

Unfortunately, these selective types of measurements can not be made in all cases and the calibration can be error prone. However, if proper validation procedures are followed, it should be possible to detect unreliable results in most cases. Nevertheless, a paucity of post-audit studies makes it impossible to ensure that unreliable or error prone results will be detected in all cases.

In addition to the selective concentration measurements to aid calibration, there are calibration procedures designed to aid in investigating loading data and avoid calibration errors. These procedures generally follow a phased approach that is described in the section on calibration procedures.

Finally, embarrassing errors can occur in the formulation of model data sets. To avoid these calibration errors, there are two methods that should be employed. First, conservation of mass should always be checked. This is done by simulating a conservative constituent such as dissolved solids or by using a hypothetical unit loading of 1, 10, or 100 concentration units to be sure that dilution, transport, and mixing are properly quantified. Second, the calibration should be compared to any analytical or simpler solution available. Section 6 provides some simple formulations that may be useful and Thomann and Mueller (1987) provide a wealth of additional information. When simple calculations are not possible, selective hand calculations using the more elaborate equations in critical areas are recommended to be sure that the modeler understands the data sets that have been formulated. A sensitivity analysis to indicate critical locations and important processes that should be checked, is suggested.

Calibration alone is not adequate to determine the predictive capability of a model for a particular estuary. To map out the range of conditions over which the model can be used to determine cause and effect relationships, one or more additional independent sets of data are required to determine whether the model is predictively valid. This testing exercise, which also is referred to as confirmation testing (Reckhow and Chapra 1983), defines the limits of usefulness of the calibrated model. Without validation testing, the calibrated model remains a description of the conditions defined by the calibration data set. The uncertainty of any projection or extrapolation of a calibrated model would be unknown unless this is estimated during the validation procedure.

In addition, the final validation is limited to the range of conditions defined by the calibration and validation data sets. The uncertainty of any projection or extrapolation outside this range also remains unknown. The validation of a calibrated model, therefore, should not be taken to infer that the model is predictively valid over the full range of conditions that can occur in an estuary. For example, a model validated over the range of typical tides and low freshwater inflow may not describe conditions that occur when large inflows and atypical tides occur. This is especially true when processes such as sediment transport and benthic exchange occur during atypical events but not during the normal, river flow and tidal events typically used to calibrate and validate the model.

To stress the limited nature of a calibrated model, validation testing is used here in place of the frequently used terminology "model verification." Strictly speaking, verification implies a comparison between model predictions and the true state of an estuary. Because the true state can only be measured and thus known only approximately, validation is a better description of what is actually done. Furthermore, many diverse modeling fields seem to refer to the procedure of initially testing a computer model on different computer systems using a benchmark set of input data as verification. In this latter case, the term verification is more appropriate because model simulations on a different computer are being compared with an exact benchmark condition derived by the developer on his original computer. For engineering purposes, these calculations are "precise enough" to serve as exact definitions.

In the past, the adequacy of model calibration and validation generally has been evaluated by visually comparing model predictions and measured data. There are statistical criteria, as well, that should be used in testing the adequacy of a calibration or validation. These will be critically reviewed in the final part of this section.

Figures 5.1 and 5.2 describe, in general terms, the calibration and validation procedure. As noted in the introductory section of this manual, waste load allocation modeling is an iterative process of collecting data, calibrating a model, collecting additional data, and attempting to validate the model. In some critically important estuaries, such as Chesapeake Bay, the Delaware Estuary, New York Harbor, and San Francis-

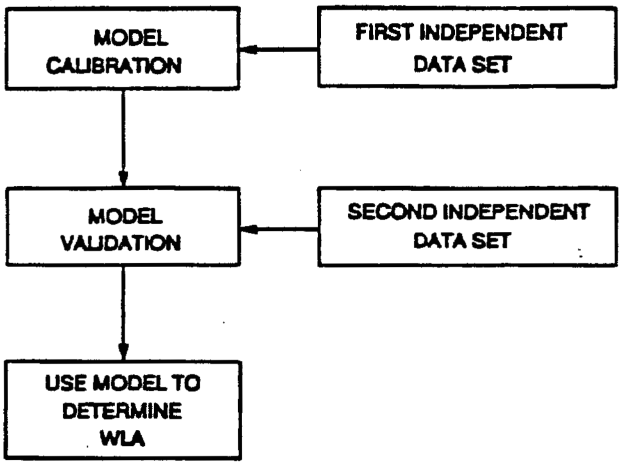


Figure 5-1. Model calibration and verification procedure.

co Bay, it is necessary to continually update assessments and waste load allocation studies. It is possible, however, to adequately validate a model and set reasonable waste loads in a short period of study (i.e., 6 to 12 months) for most smaller estuaries or for smaller sections of larger estuaries.

5.2. Model Calibration

As illustrated in Figure 5.3, sets of data are collected to define the loads and flows entering and leaving an estuary and to characterize the receiving water quality for comparison to conditions simulated by the waste load allocation model. The appropriate data collection procedures, which are equally important to developing a well calibrated model, are described in Section 4.0. The inflows, outflows, and loads entering and leaving the estuary are used to specify the model boundary conditions. These inputs to the model, along with specified model coefficients, control the simulation of receiving water quality. Calibration of the model involves a comparison of the measured and simulated receiving water quality conditions. Model coefficients are modified by trial and error until the measurements and simulations agree reasonably well (e.g., see McCutcheon 1989, Thomann and Mueller 1987). Ideally, agreement should be evaluated in terms of

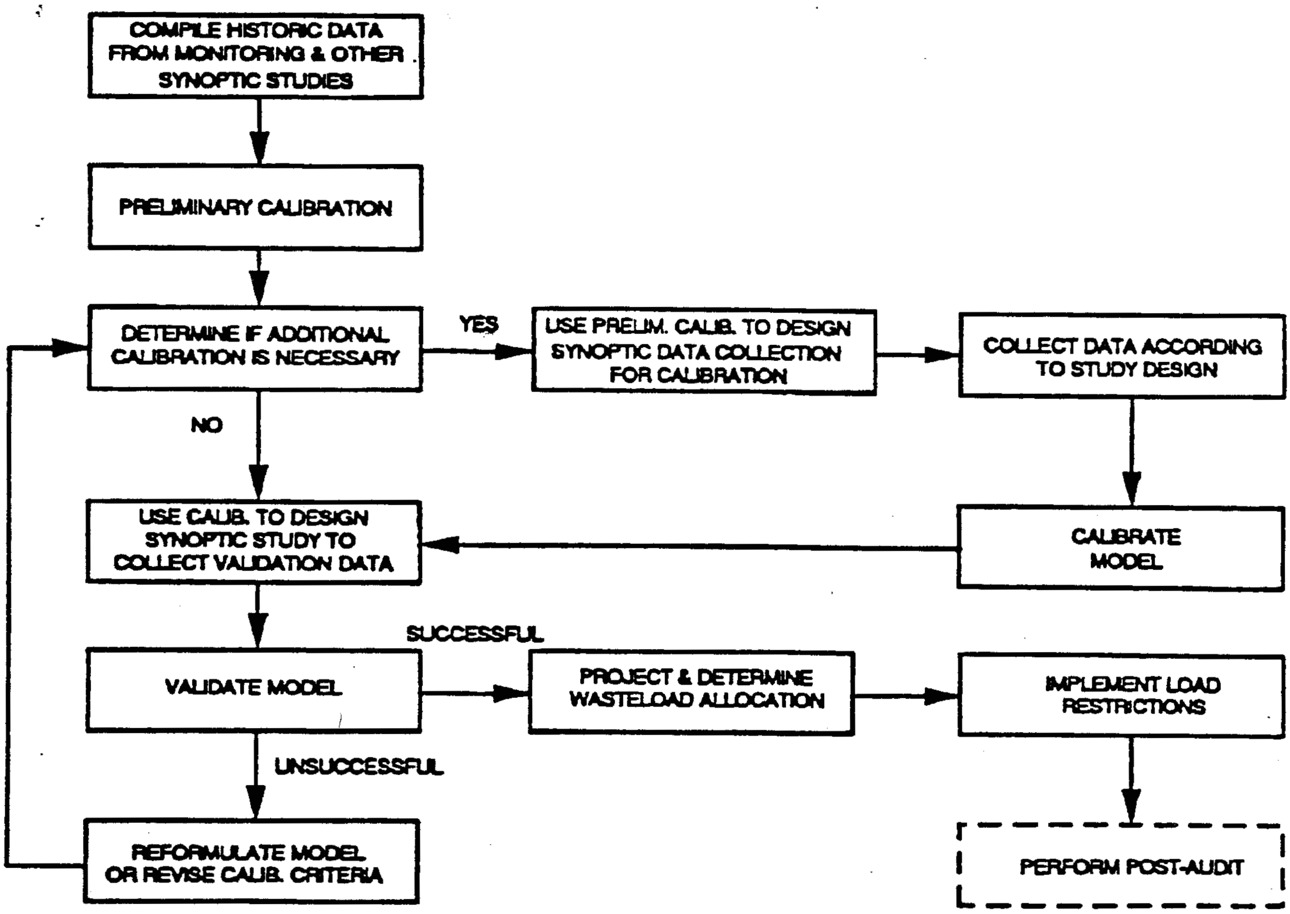


Figure 5-2. Relationship between data collection, model calibration, validation, and waste load allocation procedures.

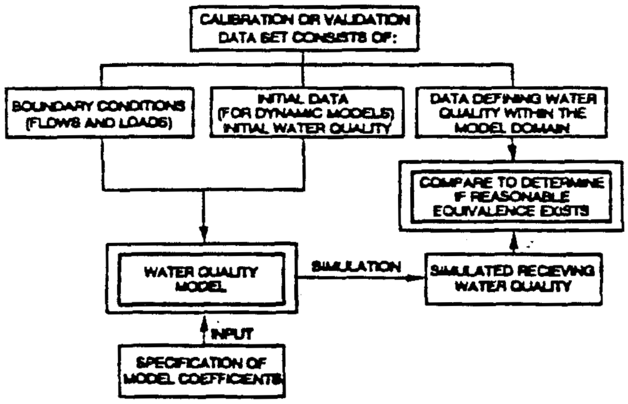


Figure 5-3. Relationship between data set components, water quality model, and set of model coefficients for model calibration.

prespecified criteria. Very little guidance is available, however, to make this fully feasible.

Occasionally, the trial and error procedure reduces to one trial of a coefficient either estimated by empirical formulations or measured. Typically this occurs when model results are not sensitive to a particular coefficient.

A number of methods (e.g., least squares and maximum likelihood) can and should be used to guide the subsequent trials of coefficients. Various statistical criteria such as least squares have been selected as the basis for schemes to select optimum sets of model coefficients. Unfortunately, use of optimization schemes still require expert judgement to weigh the importance of subsets of data being used for calibration and to establish ranges of coefficients from which to select from a given estuary. A critical limitation seems to involve a lack of knowledge about correlations between parameters that influence the selection of an optimum set. As a result, calibration by optimization is not frequently used unless extremely complex models are employed where significant time savings may be achieved.

The most useful compilations of these model formulations and range of coefficients are published in the EPA guidance manuals for conventional and toxic pollutants given in Table 5.1. In addition, guidance is available from a number of reference books (e.g., Thomann and Mueller 1987, Krenkel and Novotny 1980, McCutcheon 1989, 1990, and Rich 1973).

In general, models are calibrated in phases beginning with the selection of the model parameters and coefficients that are independent (or assumed to be independent in the formulation of the model) as shown in Table 5.2 for conventional pollutants when baroclinic circulation is not important. The final phases focus on

Table 5-1. Guidance Manuals for Rates, Constants, and Kinetics Formulations for Conventional and Toxic Pollutants

1. Bowie, G.L., Mills, W.B., Porcella, D.B., Campbell, C.L., Pagenkopf, J.R., Rupp, G.L., Johnson, K.M., Chan, P.W.H., and Gherini, S.A., **Rates, Constants, and Kinetics Formulations in Surface Water Quality Modeling**, 2nd ed., EPA 600/3-85/040, U.S. Environmental Protection Agency, Athens, Georgia, 1985.
2. Schnoor, J.L., Sato, C., McKechnie, D., and Sahoo, D., **Processes, Coefficients, and Models for Simulating Toxic Organics and Heavy Metals in Surface Waters**, EPA/600/3-87/015, U.S. Environmental Protection Agency, Athens, Georgia, 1987

Table 5-2. Outline of a General Calibration Procedure for Water Quality Models for Conventional Pollutants when Baroclinic Circulation Effects are Unimportant [McCutcheon, (1989)]

Step	Procedure
1	Calibrate hydraulics or hydrodynamics model by reproducing measurements of discharge, velocity, or stage (depth of flow) at selected sensitive locations. This involves modification of the Manning roughness coefficient, eddy viscosity coefficients, or empirical flow versus stage coefficients to predict the proper residence time through the reach of interest. Dye studies to determine time of travel or average velocity may be used in place of hydraulic measurements for some simpler models.
2	Select dispersion or mixing coefficients (or eddy diffusivities) to reproduce any dispersive mixing that may be important. Natural tracers or injected dye clouds may be monitored for this purpose.
3	Calibrate any process models such as water temperature that are not affected by any other water quality constituent.
4	Calibrate any process model affected by the processes first calibrated. In conventional models, this may include biochemical oxygen demand (BOD), fecal coliform bacteria, and nitrification.
5	Finally, calibrate all constituents or material cycles affected by any other process. In conventional models this usually means that the dissolved oxygen balance is calibrated last after biochemical oxygen demand, nitrification and photosynthesis sub-models are calibrated.

the least independent parameters as illustrated in Figure 5.4. Typically, as many as three distinct phases are involved and each phase involves the selection of a number of critical parameters and coefficients as shown in Tables 5.3, 5.4, and 5.5.

5.2.1. Phase I of Calibration

Phase I concentrates on the calibration of the hydrodynamic and mass transport models. In general, there is a complex interaction between circulation and density differences caused by gradients of salinity and temperature that must be taken into account in stratified estuaries. In vertically mixed estuaries, the

Table 5-3. **Guidance on the Selection of Model Coefficients and Parameters - Phase I**

Calibration Parameters for: Complex Model	Calibration Parameters for: Simple Model	Range of Values	Guidance Documents and References
Bottom roughness coefficient		0.010 to 0.120	Hydrodynamic model documentation [i.e. Ambrose et al. (1988)], Chow (1959), Frecnh (1985), Barnes (1972)
Eddy Viscosity: Vertical[1] Lateral[1] Horizontal		 10-2 to 10^0 cm s^{-1} 102 to 10^6 cm s^{-1} 10^2 to 10^6 cm s^{-1}	Hydrodynamic model documentation. Assumed to be the same order as the dispersion coefficient. Bowie et al. (1985), NAS (1977), Officer (1979), and Dyer (1973)
Dispersion Coefficient: Vertical Lateral[1] Horizontal[1]	Dispersion Coefficient: Vertical Lateral[1] Horizontal[1]	 10^{-2} to 10^0 cm s^{-1} 10^2 to 10^6 cm s^{-1} 10^2 to 10^6 cm s^{-1}	Bowie et al. (1985), Fisher et al. (1979), Thomann and Mueller (1987), NAS (1977), and Officer (1976)
Wind speed function		See Supplement VI	Bowie et al. (1985), Ryan and Harleman (1973), Brutsaert (1982), and McCutcheon (1989)
Surface drag coefficient		0.001 to 0.0025	O'Connor (1983)

[1] Harleman, in review, notes that these ranges are too large to be fully useful. However, the data does reflect the approximate nature of these types of models and shows the extreme variability to be expected.

interaction among salinity, temperature and circulation is usually not significant. When vertical salinity gradients are not present, vertically mixed one-and two-dimensional models are employed and these are relatively easy to calibrate. In these cases, circulation in the estuary is not as strongly controlled by changes in salinity and temperature. As a result, the hydrodynamic model can first be calibrated and then the salinity and temperature models calibrated afterwards. Model calibration for stratified estuaries involves determining bottom and surface friction coefficients (see Supplements I and II) and vertical, lateral, and horizontal eddy viscosity coefficients for the hydrodynamic model (see Supplements III and IV). The calibration of the mass transport model is achieved by properly selecting the vertical, lateral, and horizontal mass transfer coefficients (see Supplement V). The

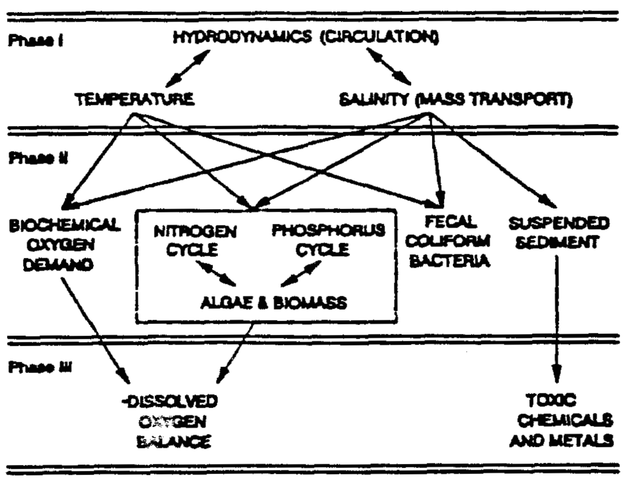


Figure 5-4. Phased calibration procedure.

calibration of the temperature model is accomplished by selection of the proper wind speed coefficients (see Supplement VI). See Table 5.3 for a listing of the coefficients that must be selected for the most general case.

Under the simplest and best conditions, however, it is possible to calibrate the circulation model and mass transport model with tracer or salinity measurements and ignore any variation in temperature. Typically, this sort of indirect calibration works well when the estuary can be simulated with a one-dimensional model but it is also the method most frequently attempted for all types of flows including complex stratified flows. Whether the indirect method is useful or not depends on the expertise of the model user and whether the waste load allocation is very sensitive to circulation patterns in the estuary. At the very least, this method should be attempted and used in preliminary model setup when simulating the estuary with whatever historic data are available to assist in planning data collection studies.

Generally, calibration procedures for hydrodynamic models are not well developed. In fact, it is not clear that the full resolution available from two- and three-dimensional models are fully useful to inexperienced modelers. As a result, precise calibrations are rarely attempted for routine waste load allocation studies. When it is necessary to precisely define complex circulation patterns due to the dynamic action of tides and wind, stratification, or coriolis effects, the modeling is usually left to experts (e.g., HYDROQUAL 1987). In part, precise calibrations are not attempted because critical circulation conditions for estuaries analogous to the critical low flow case found in streams have not been defined. For example, it is rarely obvious what

Table 5-4. Guidance on the Selection of Model Coefficients and Parameters - Phase II

Calibration Parameters for: Complex Model	Simple Model	Range of Values	Guidance Documents and References
CBOD:	CBOD:		Bowie et al. (1985)
Deoxygenation rate coefficient	Deoxygenation rate coefficient	0.05 to 0.4 d^{-1} (20°C)	
Decay rate coefficient	Decay rate coefficient	0.05 to 0.4 d^{-1} (20°C)	
Settling coefficient	Settling coefficient	approximately 0.0	
	NBOD decay rate coefficient	0.1 to 0.5 d^{-1} (20°C)	Bowie et al. (1985), Thomann and Mueller (1987)
Nitrogen transformations:			Bowie et al. (1985)
ON hydrolysis rate coefficient		0.001 to 0.14 in d^{-1} (20°C)	
Ammonification rate coefficient		0.02 to 1.3 in d^{-1} (20°C)	
Nitrification rate coefficient		0.1 to 20 in d^{-1} (20°C)	
Phosphorus transformations			Bowie et al. (1985)
$OP \rightarrow PO_4$		0.001 to 0.2 d^{-1} (20°C)	
Biomass coefficients:			Bowie et al. (1985)
Ammonia preference factor		0 to 1.0	
N half sat. constant		0.001 to 0.4 mg L^{-1}	
P half sat. constant		0.0005 to 0.08 mg L^{-1}	Thomann (1972) - Delaware Estuary
Light half sat. constant		0.1 x 10^{-5} to 20.5 x 10^{-5} W m^{-2}	
Light ext. coefficient		2.3 to 6.9 in m^{-1}	
Max growth rate coeff.		0.2 to 5 d^{-1} (20°C)	
Respiration rate coeff.		0.05 to 0.15 d^{-1} (20°C)	
Settling rate		0.05 to 0.6 m d^{-1}	
Non-predatory mortality rate		0.003 to 0.17 d^{-1}	
Zooplankton grazing rate		0.35 to 0.8 d^{-1}	
Phytoplankton stochiometry:		(% dry weight biomass)	Bowie et al. (1985) - see their table of values for various species.
Carbon		10 to 70	
Nitrogen		0.6 to 16	
Phosphorus		0.16 to 5	
Silica		20 to 50	
	Net photsynthesis rate	0.5 to 5 g O_2 m^{-2} d^{-1}	Thomann (1972), Mills et al. (1985)
	Net respiration rate	same order of magnitude as photosynthesis rate	Mills et al. (1985)
Coliform die-off rate coefficient	Coliform die-off rate coefficient	0 to 84 d^{-1}	Bowie et al. (1985), Thomann and Mueller (1987)
Settling velocity		1 to 100 m d^{-1}	Thomann in review
Resuspension velocity		0.1 to 50 m yr^{-1}	Thomann in review
Net settling velocity		0.1 to 50 cm yr^{-1}	Thomann in review

Definition of symbols and explanation of terms:

ON = organic nitrogen
ON hydrolysis = degradation of organic nitrogen to ammonia
Ammonification = oxidation of ammonia to nitrate
Nitrification = oxidation of nitrite to nitrate

Table 5-5. Guidance on the Selection of Model Coefficients and Parameters - Phase III

Calibration Parameters for: Complex Model	Calibration Parameters for: Simple Model	Range of Values	Guidance Documents and References
Sediment oxygen demand rate	Sediment oxygen demand rate	0.0 to 11 in g O_2 m^{-2} d^{-1}	Bowie et al. (1985), Krenkel and Novotny (1980)
Rearation rate coefficient	Reaeration rate coefficient	order of 0.001 to 0.1 d^{-1} or K_2 = $(depth)^{-1}d^{-1}$, depth in m	Bowie et al. (1985), Kim and Holley (1988), Thomann and Mueller (1987)
	Toxics 1st order decay coefficient	Not well defined	
Toxicant Fate Processes: Volatilization rate coefficient; Biodegradation rate coefficient; Photolysis rate coefficient; Hydrolysis rate coefficient (Acid, Neutral, Base)		See range for each individual chemical	Schnoor et al. (1987), Mills et al. (1985)
Partitioning coefficient			Thomann and Mueller (1987)
	Conservative heavy metals with settling		Thomann in review
Metals Fate Processes: Solubility constants; Chemical equilibrium constants			See data bases in MINTEQA2 model [Brown and Allison (1987)] and other geochemical speciation models, and Stumm and Morgan (1981), Schnoor et al. (1987)

Definition: K_2 = reaeration coefficient.

combination of freshwater inflow, wind conditions, tidal conditions, and storm effects represent a critical circulation condition on which the design of a sewage treatment plant should be based to provide adequate protection of water quality. Therefore, calibrations are usually based on uniformly constant roughness coefficients and literature estimates of eddy viscosity values that only attempt to capture estimates of gross circulation patterns for selected conditions. The few readily available studies (many are published in "grey literature" reports) that have explored circulation in detail, did not include sensitivity. Typically, this sort of indirect calibration works well when the estuary can be simulated with a one-dimensional model, but it is also the method most frequently attempted for all types of flow analyses to establish what combinations of conditions lead to a reasonable worst case design standard. Similarly, the sensitivity of water quality to hydrodynamic conditions has not been explored in any study that leading experts are aware of. (conclusion of the January 1988 Workshop 3: Hydrodynamic and Water Quality Model Interfacing and Workshop 4: Long Term Modeling of Chesapeake Bay, Baltimore, Maryland, U.S. Army Corps of Engineers and U.S. Environmental Protection Agency).

The best studies attempt to collect current velocity data for calibration but questions remain about the appropriate procedure for averaging data for comparison with model results. As a result, opportunities remain for the development of innovative approaches to data collection and interpretation for comparison with model simulations. Generally, water elevations measured at a very few locations (one to three) are the only data readily available for direct calibration (e.g., Thatcher and Harleman 1981). Typically, circulation models are indirectly calibrated from salinity or conservative tracer measurements that also must be used to calibrate the mass transport model as mentioned above. Indirect calibration can result in an imprecise calibration of both the circulation and mass transport algorithms but this is not a severe drawback unless the critical water quality components of the waste load allocation model are sensitive to small changes in circulation and mass transport. In addition, hydrodynamic models are more firmly based on first principles than other water quality model components. As a result, there is a greater possibility of making valid hydrodynamic predictions without extensive calibration.

In contrast with two- and three-dimensional models, a number of one-dimensional hydrodynamic models have been determined to be generally useful (e.g., Ambrose et al. 1988, Ambrose and Roesch 1982, and Thatcher and Harleman 1981). These one-dimensional models are occasionally calibrated with current velocity and water surface elevation data but more often are calibrated by indirect means. The dominant calibration parameter for a one-dimensional model is the roughness coefficient (the Manning n or Chezy C), which is relatively easy to select. Supplement I also reviews the selection procedure for the Manning n that is used in simpler one-dimensional models.

5.2.2. Phase II of Calibration

Phase II involves the selection of coliform die-off coefficients, settling and re-suspension velocities for suspended sediment, BOD coefficients, and the set of coefficients describing the nutrient cycles and photosynthesis. The selection of die-off coefficients is relatively straightforward compared with other phases of the calibration (see Supplement VII, and Thomann and Mueller 1987, and Bowie et al. 1985). Derivation of parameters describing sediment transport and BOD is somewhat more involved. The calibration of nutrient and phytoplankton models requires some skill and expertise because of the complexity of the potential interactions between a number of the components of the cycles involved.

Suspended sediment and BOD models are somewhat more difficult to calibrate because the processes can not be fully defined by measurement techniques readily available for the collection of calibration data. Suspended sediment is continually exchanged with bottom deposits and this exchange can be relatively important in tracing the fate of nutrients and sorbed contaminants. Unfortunately, it is only feasible at present to measure changes in suspended sediment at various locations over time and to measure long term net deposition or erosion of sediments. The limited guidance available for calibrating simple sediment transport models is presented in Supplement VIII.

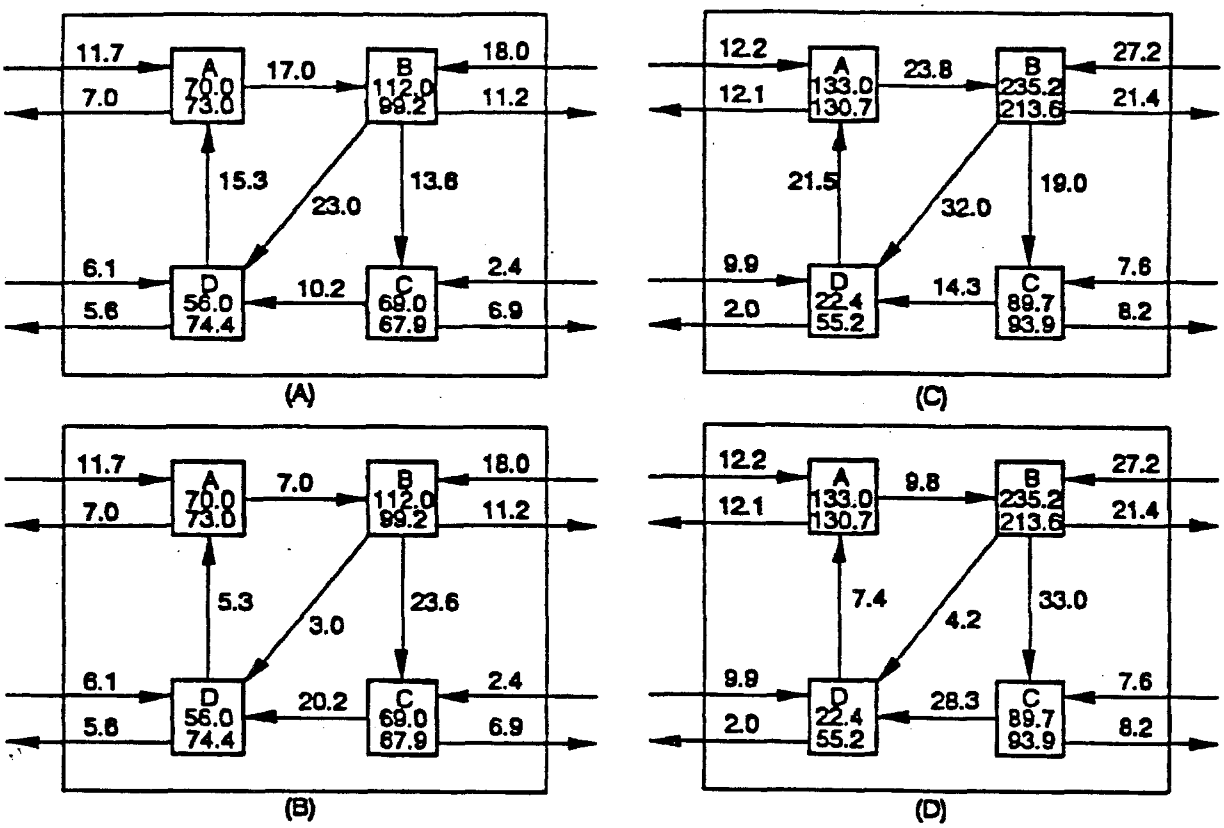
The calibration of a model for BOD is complicated if settling and sorption to organic material is occurring along with biodegradation. If only water column BOD measurements are available, it is difficult to determine the relative importance of deoxygenation, settling, and adsorption of dissolved BOD on the dissolved oxygen balance. Settling is usually not important, however, because of recent advances (since the late 1960s) in regulating organic solids in waste effluents. This is especially true away from a localized mixing zone at the point of discharge where some flocculation and settling may occur. In addition, the relatively large depths of estuaries preclude rapid adsorption of dissolved BOD like that observed in streams because of the limited surface area available. Also, brackish waters tend to slow biotic reactions and growth which should slow the uptake of dissolved organic carbon. Therefore, calibration of BOD models frequently can be a simple matter of accounting for the decay of BOD measured in the water column. Recommendations for calibration of a BOD model are given in Supplement IX.

The effect of nitrification can be modeled in two ways. First, simple nitrogenous BOD (NBOD) models have been utilized. Second, and most useful, are nitrification models of organic nitrogen, ammonia, nitrite, and nitrate. NBOD models are typically only useful when nitrification is relatively unimportant in the dissolved oxygen balance. Supplement X gives useful guidance for the implementation of an NBOD model. Supplement XI gives guidance on the selection of nitrification rate constants and parameters. The nitrification model is more complex but this complexity is well justified by the existence of well defined measurement techniques and calibration procedures. Nutrient and phytoplankton models typically involve several separate major components and a number of minor components that are frequently ignored or lumped in with the major components. The most difficult problem faced in the calibration process is that a unique set of coefficients is difficult to derive. The limited guidance available on the calibration of nitrogen and phosphorus models is given in Supplements XI and XII.

Wlosinski (1984) illustrates this problem with a simple example involving an interactive four component model shown in Figure 5.5. This example is somewhat abstract but it shows that exactly the same values of the state variables can be computed in two cases with significantly different process rates controlling the magnitude of mass transfer between environmental components. In addition, Wlosinski shows that validation testing also can fail to detect a problem unless the data set is significantly different from the calibration data. Therefore, he recommends, as we emphasize in this section, that models be carefully validated and suggests that as many process rate measurements be made as possible. These are measurements of gas transfer, benthic exchange, and degradation rates, to name a few of the most important. Clearly, it is not possible to uniquely describe an estuarine water quality system without at least one process rate measurement.

5.2.3. Phase III of Calibration

The final phase of calibration can be either difficult or extremely easy depending on how well other components have been calibrated and whether process measurements such as the reaeration rate and sediment oxygen demand rates have been measured as part of the calibration data collection study. Typically, this final phase highlights weaknesses in the prior calibration steps that must be addressed by repeating some steps to achieve a more consistent overall calibration. In fact, it is more useful to attempt a quick step through the calibration procedure to obtain a



EXAMPLE OF TWO MODELS BEING CALIBRATED ON SAME SYSTEM: A) MODEL 1; (B) MODEL 2

EXAMPLE OF TWO MODELS BEING VALIDATED ON SAME SYSTEM: (C) MODEL 1; (D) MODEL 2

Figure 5-5. Example showing that calibration is not unique unless material transformation rates are specified and that validation should be performed with significantly different data sets [Wlonsinski (1984)].

preliminary indication of which parameters and coefficients may be the most important. This assessment can be based on a preliminary sensitivity analysis.

At this stage in the calibration of a eutrophication and dissolved oxygen model, the available guidance is relatively straightforward. Supplements XIII, XIV and XV describe methods of estimating reaeration coefficients and rates of sediment oxygen demand. Once these values are initially selected, it becomes a matter of making different trials until model simulations and measurements are in reasonable agreement.

Available guidance for calibration of toxic chemical models is not as clear. Generally, it is not always clear what types of models should be implemented and it is difficult to ascertain beforehand what measurements may be required to form a comprehensive data set for calibration and validation. At this time, the best guidance is contained in Schnoor et al. (1987).

Schnoor et al. (1987) review formulations of the fate processes for organic chemicals and heavy metals. They review the effects of biodegradation, hydrolysis, oxidation, photolysis, volatilization, sorption, and bioconcentration for organic contaminants and compile rate constants for these processes that can be used in model calibration.

Schnoor et al. (1987) also review the transformation and transport mechanisms affecting selected metals. These include cadium, arsenic, mercury, selenium, lead, barium, zinc, and copper. In addition, screening level information can be obtained from metals speciation models (Brown and Allison 1987).

In review, Robert Thomann recommends treating heavy metals as conservative constituents except for partitioning with sediments when crude estimates of a distribution coefficient can be used to estimate dissolved concentrations. Estimates of the distribution coefficient can be obtained from Schnoor et al. (1987) or Thomann and Mueller (1987). Geochemical speciation models such as MINTEQA2 (Brown and Allison 1987) can be used to estimate distribution coefficients (when dissolved solids are not very high – i.e., applicable for fresh or brackish waters but not sea waters) in addition to being used to determine potential mobility as indicated above.

5.3. Model Validation

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

Validation testing is performed with an independent data set collected during a second field study. The field study may occur before or after the collection of calibration data. For the best results, however, it is useful to collect the validation data after the model has been calibrated. This schedule of calibration and validation ensures that the calibration parameters are fully independent of the validation data. To extend the range of conditions over which the calibrated model is valid, however, it may be useful to save the initial study for validation testing if it is expected that data collected at a later date will provide a less severe test of the calibrated model.

At present, it is very difficult to assemble the necessary resources to conduct the desired number of surveys. Therefore, it is important that surveys be scheduled in an innovative manner and the choice of calibration and validation data sets remain flexible in order to make the test of the calibrated model as severe as possible.

Many studies are faced with severely limited resources for sampling and laboratory analysis that preclude collection of more than one set of data. If this highly undesirable circumstance occurs, the historic data should be investigated to determine whether the model can be calibrated *a priori* and validated with one set of data or *vice versa*. In any event, it is very important that both calibration and validation data be defined even if this involves splitting a single data set (a data set divided into two data sets by assigning every other datum or set of data in each time series, to separate data sets or by dividing time series data into sets covering different time periods as done by Ambrose and Roesch (1982) for calibration to selective conditions).

If a split data set is used, however, it must be clearly noted that these types of limited studies are not fully useful. Wlosinski (1985) shows that the likelihood of being unable to detect a poorly selected set of coefficients is quite low using split data sets.

Too many times, limited studies only attempt calibration. This, in effect, limits the study to describing the conditions during the calibration data collection period and increases the uncertainty associated with the waste load allocation. In fact, uncertainty can not be reliably assessed.

Once the validation tests are concluded, Reckhow and Chapra (1983) recommend that the model be recalibrated to obtain the overall optimum calibration. This should improve the overall predictions but it should not be used as a shortcut to avoid rigorous validation testing. Overall optimum calibration can be achieved by minimizing the least squares error for all data available in multiple sets or by obtaining the best overall fit between predictions and measurements from visual inspection.

5.4. Model Testing

During and after the calibration and validation of a model, at least two types of testing are important. First, throughout the calibration procedure, a sensitivity test provides a method to determine which parameters and coefficients are the most important. Second, there are a number of statistical tests that are useful for defining when adequate agreement has been obtained between model simulations and measured conditions.

The sensitivity analysis is simply an investigation of how much influence changes in model coefficients have on simulated results. Typically, important coefficients, parameters, boundary conditions, and initial conditions are varied by a positive or negative constant percentage to see what effect the change has on critical predictions. Values of ±1, ±10, and ±50 percent have been used frequently. The coefficients and parameters are changed one at a time and the effects are typically ranked to show which parameters have the most influence and which have the least influence.

A sensitivity analysis also is useful when applied to a preliminary calibration of a model using historic or estimated conditions. In this case, the ranking can be used to determine which coefficients and parameters should be measured and which can be estimated. For example, if a model is sensitive to SOD rates, these should be measured rather than estimated. If other parameters like the wind speed function have little influence, very little effort should be expended to estimate its exact form.

The second type of testing involves assessment of the goodness of fit for model simulations compared with measurement of important water quality parameters. In addition to making a visual assessment, a number of statistical tests have proven useful (Ambrose and Roesch 1982, Thomann 1982, Beck 1987, Beck 1985, Southerland et al. 1984). These include:

1. Root mean square error,
2. Relative error,
3. Regression analysis,
4. Comparison of means, and
5. Other techniques.

Recent studies of heuristic methods (e.g., "rules of thumb") for the development of expert systems indicate that a visual fit of model predictions to measured data can quite accurately be used to obtain accurate calibrations, especially if performed by experts. However, a number of useful statistical criteria can be employed to obtain an optimum fit and these avoid any bias that may be introduced by inexperienced modelers.

5.4.1. Root Mean Square Error

The most widely used criterion to evaluate the agreement between model predictions and measurements is perhaps the root mean square (rms) error or standard error of the estimate (Ambrose and Roesh 1982) defined as

$$rms = \left[\frac{\Sigma(C_m - C_s)^2}{N}\right]^{0.5} \qquad (5.1)$$

where

C_s = simulated concentration or state variable
C_m = measured concentration or state variable
N = number of measurements

The rms error can be used to compute simultaneous discrepancies at a number of points or it can be used to compute discrepancies between measurements and predictions at a single point over time (Thomann 1982). Ensemble or global rms errors can be computed for a series of measurements at multiple points over time as

$$rms_g = \left[\frac{\Sigma\,(C_m - C_s)^2}{N_i}\right]^{0.5} \qquad (5.2)$$

where

N_i = the total number of measurements at every site over all periods of time.

Equation (5.2) is frequently useful for obtaining the best overall fit between a model and a number of different data sets where each measurement is considered to be equally valid. For example, this statistic would be useful for obtaining an overall calibration for two or more sets of data containing different numbers of measurements that are all equally accurate. Different weighting schemes could be applied if measurements were of differing accuracy (i.e., when a less accurate dissolved oxygen meter is used in a different part of the estuary or during a different study). Beck (1987) discusses these schemes and the elements of engineering judgement involved.

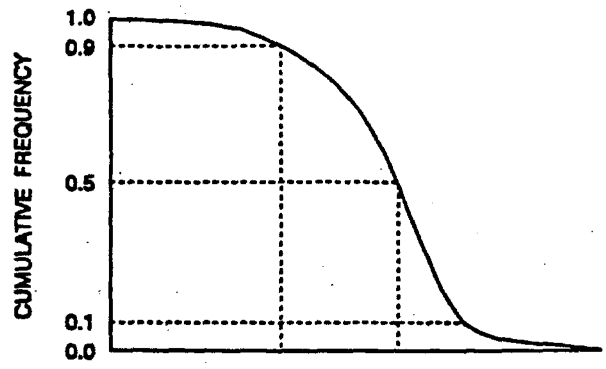


Figure 5-6. Cumulative frequency diagram.

When the rms error is expressed as a ratio to a spatial or temporal mean, the resulting statistic, which is the coefficient of variation (Kennedy and Neville 1976), represents a second type of relative error that expresses relative discrepancy. This type of relative rms error can be useful for obtaining an ensemble statistic to obtain the best overall fit for composite sets of data where each individual measurement may not be comparable between two or more separate sets of data. For example, one data set may contain more measurements that document greater dynamic uncertainty that should not be overweighted.

In general, the use of the rms error assumes that all discrepancies are of the same order and this is usually true over a limited range of conditions. However, calibration over a more extensive range where discrepancies between model predictions and measurements may be proportional to the magnitude of the measurement, other statistics (e.g., relative error) will be more appropriate. Finally, the rms error has at least one disadvantage (Thomann 1982). It is not readily evident how a pooled statistic for all state variables can be computed to assess over all model credibility.

5.4.2. Relative Error

When discrepancies between model simulations and measurements are not uniform over parts of the estuary or with time, the relative error may be a more appropriate statistic for testing calibration or validation. The relative error is defined as (Thomann 1982)

$$e = \frac{|\overline{C_m} - \overline{C_s}|}{\overline{C_m}} \tag{5.3}$$

where the overbars denote the average measured or simulated valued. Averages are performed over multiple sites or over time and cumulative frequency of error can be computed (Thomann 1982). The cumulative frequency (see for example Figure 5.6) can be used to estimate the median error and various percentiles such as the 10th and 90th exceedance frequencies. Southerland et al. (1984) notes that the 50th percentile of median error is usually reported in waste load allocations since this is the most easily understood value. The relative error behaves poorly for small values of measurements if discrepancies are not proportional to the magnitude of the measurement (i.e., small values of C_m magnify discrepancies) and if $C_m > C_s$, (since the maximum relative error is usually taken to be 100 percent). Therefore, the relative error is best for computing composite statistics when discrepancies are not constant as may occur when calibration over an extensive range is attempted.

Thomann (1982) and Ambrose and Roesch (1982) seem to offer the best available guidance on what relative errors may be appropriate to acnieve adequate estuarine dissolved oxygen model calibration. In general, median relative errors should be 15 percent or less. Values of the relative error obtained for a number of estuaries by Thomann (1982) and Ambrose and Roesch (1982) are given in Table 5.6. Note that Ambrose and Roesch define the relative error without the absolute brackets as

$$e = \frac{\overline{C_m} - \overline{C_s}}{\overline{C_m}} \tag{5.4}$$

Table 5-6. Relative Error in a Number of Estuarine Model Calibrations for Dissolved Oxygen. [Thomann (1982) and Ambrose and Roesch (1982)]

Estuary	Relative Error $\frac{\lvert\overline{C_m}-\overline{C_s}\rvert}{\overline{C_m}}$	Relative Error $\frac{\overline{C_m}-\overline{C_s}}{\overline{C_m}}$
New York Harbor	5% to 35 %	
Manhasset Bay, NY	5%	
Wicomico Estuary, MY	58%	
Savannah Estuary, GA	15%	
San Joaquin Delta, CA	10%	
Potomac Estuary, MY		-3% to -1%
Delaware Estuary, PA		1%

so that on average, values of this statistic are smaller than or equal to the values obtained from Equation (5.3).

5.4.3. Regression Analysis

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

$$\overline{C_m} = a + b\,\overline{C_s} + \varepsilon \tag{5.5}$$

where

a = intercept value

b = slope of the regression line

ε = the error in measurement mean, C_m.

The standard linear regression statistics computed from Equation (5.5) provide a number of insights into the goodness of fit for a calibration (Thomann 1982, Southerland et al. 1984). These include:

1. The square of the correlation coefficient, r^2 (measure of the percent of the variance accounted for) between measured and predicted values,

2. The standard error of estimate (Kennedy and Neville 1976), representing residual error between model and data,

3. The slope estimate, b, and intercept, a, and

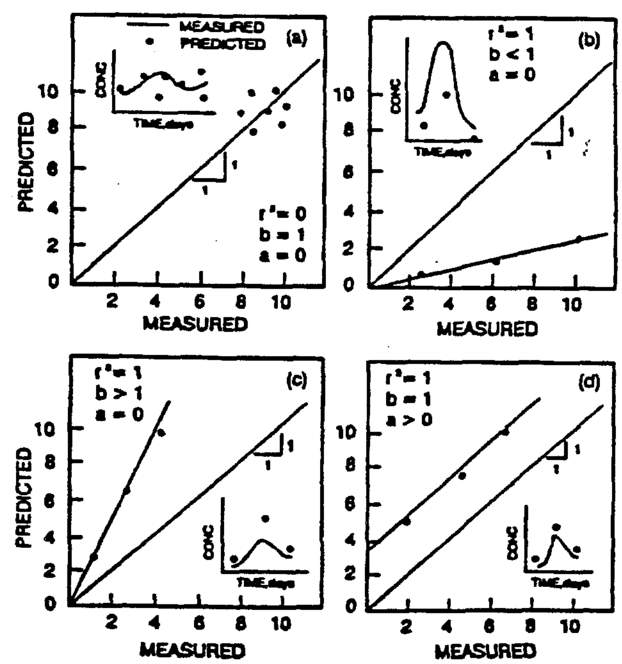


Figure 5-7. Types of bias and systematic error determined by regression analysis [(O'Connor (1979), Thomann (1982), and NCASI (1982)].

Table 5-7. Hydrodynamic Model Error Statistics for the Delaware Estuary [Ambrose and Roesch (1982)]

Tidal Response Variables	N	Calculated Errors				Regression Statistics		
		E	RE	SE	CV	a	b	r
Tidal range (m)	15	-0.012	-0.00	0.093	0.02	1.03	-0.06	0.98
High water arrival (min)	15	18.4	-0.09	19.9	0.10	0.94	-6.69	1.00
Low water arrival (min)	15	-1.27	-0.01	7.6	0.03	0.99	0.32	1.00
Ebb flow (min)	12	-8.3	-0.02	22.9	0.05	0.42	25	0.94
Max flood velocity (m/s)	12	-0.20	-0.21	0.28	0.29	0.56	0.22	0.69
Max ebb velocity (m/s)	12	-0.37	-0.34	0.40	0.37	0.85	-0.21	0.70

Table 5-8. Hydrodynamic Model Error Statistics for the Potomac Estuary [Ambrose and Roesch (1982)]

Tidal Response Variables	N	Calculated Errors				Regression Statistics		
		E	RE	SE	CV	a	b	r
Tidal range (m)	82	-0.001	-0.00	0.036	0.06	0.92	0.046	0.98
High water arrival (min)	82	0.076	0.02	0.27	0.07	0.97	0.03	0.99
Low water arrival (min)	82	0.025	0.01	0.22	0.05	0.98	0.07	1.00
Max flood velocity (m/s)	15	-0.01	-0.04	0.16	0.23	0.37	0.44	0.54
Max ebb velocity (m/s)	15	0.03	0.10	0.15	0.23	0.40	0.37	0.67

4. The test of significance for the slope and intercept.

Figure 5.7 from O'Connor (1979), Thomann (1982), and NCASI (1982) illustrates the insight available from a regression analysis. Figure 5.7(a) shows that an unbiased estimate can result even when a correlation between measured and predicted data does not exist. Figure 5.7(b), (c) and (d) show that a very good correlation can occur when a constant fractional bias ($b > 1$ or $b < 1$) and a constant bias ($a > 0$) occurs. The slope of the regression curve indicates how well trends can be projected with the calibrated model and the intercept of the regression indicates if any systematic error is present in the calibrated model. The test of significance of the slope and intercept to detect the probable existence of any error in trend or systematic errors should be based on the null hypothesis that $b = 1$ and $a = 0$. The test statistics ($b - 1/s_b$) and a/s_a are distributed as the student's t distribution with n-2 degrees of freedom. See standard texts such as Kennedy and Neville (1976) for formulas to compute the standard deviation of the slope and intercept, s_b and s_a. Thomann recommends a "two-tailed" t test employing a 5 percent level of significance. This yields a critical t value of approximately 2 for the rejection of the null hypothesis.

5.4.4. Comparison of Means

A third criterion for agreement between measured and predicted values can be derived from a simple test of the difference between the computed and measured mean values (Thomann 1982). The most general test statistic for this purpose is based on the Student's t probability density function (see Kennedy and Neville 1976)

$$t = \frac{\overline{C_m} - \overline{C_s} - d}{s_d} \qquad (5.6)$$

where

d = true difference between model predictions and measurements (normally zero)

s_d = the standard deviation of the difference given by a pooled variance of measured and predicted variability where if these variances are assumed equal,

$$s_d = (2 s_x')^{1/2} \qquad (5.7)$$

where

s_x' = standard error of estimate of the measured data given by the standard deviation, s_x, divided by the number of measurements

$$(s_x')^2 = (s_x)^2/N \qquad (5.8)$$

The use of a test like this comparison of means requires that the computed statistic be compared with a statistic value based on a level of significance or probability. Typically, a 5 percent level is used. At least one stream study (NCASI 1982) has required that at least 95 percent of the data fall within the 95 percent confidence interval (5 percent level of significance) to achieve calibration. Less stringent criteria were used to evaluate the validation of the model for the same stream. These criteria were that 60 percent of data had to fall within the 95 percent confidence interval. Where

Table 5-9. Transport Model Error Statistics for the Delaware Estuary [Ambrose and Roesch (1982)]

Tidal Response Variables		Calculated Errors				Regression Statistics		
	N	E	RE	SE	CV	a	b	r
Chloride concentration (mg/L)	35	-140.	-0.10	440.	0.31	0.97	-98.0	0.97
Movement of 500 mg/L Isochlor (km)	5	-1.9	-0.22	2.8	0.33	0.78	-0.05	0.99
Peak dye concentration (ug/L)								
All data:	14	0.03	0.09	0.10	0.30	0.82	0.09	0.82
Period 1:	7	0.06	0.14	0.14	0.32	0.52	0.27	0.62
Period 2:	7	0.01	0.05	0.03	0.14	0.76	0.07	0.92
Movement of dye peak (km)								
All data:	14	3.4	0.26	6.0	0.45	1.12	1.8	0.96
Period 1:	7	1.6	0.54	5.1	1.73	0.15	4.2	0.44
Period 2:	7	5.0	0.21	6.6	0.28	1.26	-1.1	0.98
Width of 0.1 ug/L dye isocline (km)								
All data:	14	1.3	0.05	3.2	0.13	0.83	5.5	0.90
Period 1:	7	1.0	0.04	2.3	0.10	0.84	4.5	0.96
Period 2:	7	1.6	0.06	4.0	0.14	0.38	20.0	0.47

Table 5-10. Transport Model Error Statistics for the Potomac Estuary [Ambrose and Roesch (1982)]

Tidal Response Variables		Calculated Errors				Regression Statistics		
	N	E	RE	SE	CV	a	b	r
Chloride concentration (mg/L)	37	-85.	-0.02	200.	0.05	0.95	300.	1.00
Dye concentration (ug/L)								
All data:	189	0.00	0.00	0.12	0.44	0.69	0.08	0.84
Period 1:	50	0.11	0.27	0.18	0.44	0.68	0.05	0.81
Period 2:	139	-0.03	-0.14	0.08	0.37	0.85	0.06	0.85
Peak dye concentration (ug/L)	14	-0.01	-0.01	0.15	0.22	0.96	0.02	0.91
Movement of dye peak (km)	14	-0.9	-0.14	1.4	0.22	0.98	1.0	0.97
Width of 0.1 ug/L dye isocline (km)	10	1.9	0.10	1.3	0.07	0.66	4.5	0.96

a large number of data are available, a statistic based on the gaussian or normal distribution can be used in place of the Student's t distribution.

5.4.5. *Other Techniques*

Beck (1987) and Southerland et al. (1984) describe other techniques that can be used to aid in parameter estimation to calibrate models. Generally, these methods require some knowledge of the distribution of discrepancies between measurements and predictions or involve tests to determine the distribution. Methods requiring *a priori* knowledge of the distributions include: 1) maximum likelihood estimator, and 2) Bayesian estimator. Southerland et al. (1984) note that the Kolmogorov-Smirnov one sided test can be used to evaluate whether a significant difference exists between an observed distribution and a normal distribution. If the distribution is normal, the F-test (Kennedy and Neville 1976) of the variances of measurements and predictions is a measure of the goodness of fit. In addition, the Kolmogorov-Smirnov two sided test can be used to evaluate goodness of fit.

5.4.6. *Guidance on Statistical Criteria for Calibration and Validation*

Few studies have included calculations of statistical criteria to guide model calibration and validation and what work that is available in engineering reports has not been adequately compiled. An exception of note are the studies of the Potomac and Delaware Estuaries by Ambrose and Roesch (1982).

The work of Ambrose and Roesch (1982) is important because it presents benchmarks to which other calibrations can be compared and evaluated. In this regard, these data are very similar to the compilation of error statistics compiled by Thomann (1982) to define how well a calibrated model should simulate dissolved oxygen. Thomann's guidance only covers relative error statistics. Ambrose and Roesch define average errors, relative errors, root mean square errors, coefficient of variation, regression intercept, regression slope, and correlation coefficients but only for two estuaries. Nevertheless, the Potomac and Delaware Estuaries are among the most important East

Table 5-11. Water Quality Model Error Statistics for the Delaware Estuary [Ambrose and Roesch (1982)]

Quality Response Variables	N	Calculated Errors E	RE	SE	CV	Regression Statistics a	b	r
(a) Median Concentrations (mg/L)[a]								
Dissolved Oxygen	36	-0.15	-0.04	0.69	0.18	0.84	0.44	0.93
BOD	8	-0.70	-0.11	0.97	0.15	0.84	0.37	0.93
Ammonia-N	36	0.05	-0.10	0.16	0.33	0.90	0.10	0.91
Nitrate-N	36	-0.11	-0.08	0.24	0.17	0.90	0.04	0.91
Organic-N	36	-0.11	-0.19	0.21	0.37	0.14	0.39	0.27
(b) DO categories								
Zone 2 (mg/L)	9	-0.21	-0.04	0.50	0.10	0.78	0.90	0.91
Zone 3 (mg/L)	9	0.13	0.06	0.66	0.28	1.21	-0.38	0.78
Zone 4 (mg/L)	9	-0.10	-0.04	0.82	0.32	0.82	0.35	0.86
Zone 5 (mg/L)	9	-0.41	-0.08	0.73	0.15	0.74	0.87	0.92
Calibration (mg/L)	16	-0.06	-0.02	0.53	0.14	0.88	0.39	0.95
Verification (mg/L)	20	-0.22	-0.06	0.79	0.21	0.81	0.47	0.92
DO Minimum[b]	9	-0.07	-0.05	0.55	0.41	1.54	-0.79	0.78
2 mg/L Reach Length (km)[c]	9	-2.7	-0.13	6.0	0.28	0.90	-0.64	0.89
4 mg/L Reach Length (km)[c]	9	2.1	0.04	9.3	0.16	1.04	-0.16	0.86

[a] Concentrations are median values by river zone (> 30km) and survey period (9 total).
[b] Median concentrations during survey at minimum or maximum location.
[c] River kilometers in which concentration exceeds or falls below indicated value.

Table 5-12. Water Quality Model Error Statistics for the Potomac Estuary, 1965-1975 [Amborose and Roesch (1982)]

Quality Response Variables	N	Calculated Errors E	RE	SE	CV	Regression Statistics a	b	r
(a) Median Concentrations								
DO (mg/L)	32	-0.04	-0.01	1.02	0.17	0.80	1.12	0.86
NH_3 (mg/L)	41	0.02	0.02	0.27	0.31	1.01	0.01	0.95
NO_3 (mg/L)	39	0.05	0.07	0.18	0.26	0.79	0.21	0.90
TPO (mg/L) (as PO_4)	40	0.01	0.01	0.20	0.16	1.03	-0.03	0.98
CHL (ug/L)	31	2.7	0.04	19.3	0.27	0.92	8.70	0.87
(b) Extreme Concentration[b]								
DO Min. (mg/L)	9	-0.02	-0.01	0.35	0.23	1.08	-0.15	0.93
NH_3 Max. (mg/L)	15	-0.02	-0.01	0.20	0.11	0.91	0.15	0.96
NO_3 Max. (mg/L)	12	-0.11	-0.09	0.25	0.20	0.85	0.08	0.93
TPO Max. (mg/L, as PO_4)	14	-0.15	-0.05	0.30	0.10	1.00	-0.16	0.97
CHL Max. (ug/L)	8	-4.1	0.03	6.1	0.05	1.02	-7.1	0.99
(c) Reach Length[c]								
DO < 5 mg/L	9	-2.1	-0.10	4.3	0.20	0.81	2.1	0.78
DO < 3 mg/L	9	-1.1	-0.11	3.2	0.33	0.66	2.2	0.70
NH_3 > 1 mg/L	15	1.7	0.08	6.8	0.32	0.93	3.2	0.94
NO_3 > 1 mg/L	12	-0.3	-0.02	6.6	0.46	0.91	1.0	0.95
TPO > 1 mg/L (as PO_4)	14	0.0	0.0	8.6	0.23	0.80	7.6	0.79
CHL > 100 ug/L	8	2.2	0.10	5.3	0.25	1.11	-4.5	0.95

[a] Concentrations are median values by river segment (16-26 km) and survey period.
[b] Median concentrations during survey at minimum or maximum location.
[c] River kilometers in which concentration exceeds or falls below indicated value.

Coast estuaries and seem to be quite representative of drowned river valley types.

Ambrose and Roesch (1982) give average errors (E), relative errors (RE) [note that Equation (5.4) and not Equation (5.3) is used by Ambrose and Roesch], root mean square errors (SE), coefficient of variation (CV), regression intercept (a), regression slope (b), and correlation coefficients (r) in Tables 5.7, 5.8, 5.9, 5.10, 5.11, 5.12, 5.13 and 5.14. Tables 5.7 and 5.8 present error statistics from the calibration of a hydrodynamics model for the Delaware and Potomac estuaries. Tables 5.9 and 5.10 present error statistics from the calibration of a transport model for the Delaware and Potomac

Table 5-13. Chlorophyll-a Model Error Statistics for the Potomac Estuary, 1977-78 [Ambrose and Roesch (1982)]

Quality Response Variables		Calculated Errors				Regression Statistics		
	N	E	RE	SE	CV	a	b	r
Median concentration (ug/L)[a]	32	12.2	0.16	53.2	0.69	0.82	26.2	0.69
Peak concentration (ug/L)	8	11.3	0.07	35.1	0.23	1.16	-14.2	0.94
Peak Location (km)[b]	8	-4.8	-0.15	17.7	0.55	0.14	22.9	0.09
100 ug/L reach length (km)[c]	8	2.8	0.11	10.9	0.42	0.86	6.5	0.89

[a] Concentrations are median values by river segment (16-26 km) and survey period.
[b] Distance of peak concentration below Blue Plains Sewage Treatment Plant (river kilometer 16).
[c] River kilometers in which concentration exceeds 100 ug/L.

Table 5-14. Water Quality Model Error Statistics for the Potomac Estuary, 1977-1978 [Ambrose and Roesch (1982)]

Quality Response Variables		Calculated Errors				Regression Statistics		
	N	E	RE	SE	CV	a	b	r
(a) Median Concentrations (mg/L)								
DO	32	-0.20	-0.03	1.15	0.16	0.54	3.00	0.77
CBOD	29	-1.00	-0.31	1.57	0.48	0.25	1.47	0.33
NH_3	29	-0.11	-0.45	0.26	1.07	0.38	0.04	0.59
NO_3	40	-0.02	-0.03	0.15	0.24	0.85	0.08	0.97
(b) Extreme Concentration[b] (mg/L)								
DO Min	8	-0.03	-0.01	0.86	0.25	0.70	0.99	0.62
CBOD Max	8	-0.26	-0.04	1.92	0.32	1.30	-2.09	0.66
NH_3 Max	10	0.04	0.04	0.14	0.13	0.89	0.15	0.95
NO_3 Max	10	-0.08	-0.05	0.18	0.11	0.90	0.10	0.85
(c) Extreme Location[c] (km)								
DO Min	8	-1.2	-0.10	3.7	0.31	1.02	-1.4	0.99
CBOD Max	8	-6.0	-0.82	10.5	1.45	0.01	1.1	0.04
NH_3 Max	10	-1.4	-0.54	6.9	2.67	-0.03	1.2	-0.11
NO_3 Max	10	-2.4	-0.31	5.5	0.70	0.71	-0.2	0.89
(d) Reach Length[d] (km)								
DO < 5 mg/L	8	-3.2	-0.22	5.4	0.37	0.66	1.7	0.97
DO < 3 mg/L	8	-0.4	-0.25	2.7	1.66	0.70	0.8	0.53
CBOD > 4 mg/L	8	-12.7	-0.65	17.7	0.90	0.21	3.0	0.64
NH_3 > 1 mg/L	10	-0.2	-0.07	1.1	0.39	0.84	0.3	0.95
NH_3 > .5 mg/L	10	0.0	0.0	2.4	0.30	0.83	1.4	0.92
NO_3 > 1 mg/L	10	-2.7	-0.11	6.3	0.26	-0.03	21.9	-0.03

[a] Concentrations are median values by river segment (16-26 km) and survey period.
[b] Median concentrations during survey at minimum or maximum location.
[c] Distance of extreme concentration below Blue Plains Sewage Treatment Plant (river kilometer 16)
[d] River kilometers in which concentration exceeds or falls below indicated value.

Estuaries, respectively. Tables 5.11, 5.12, 5.13, and 5.14 provide error statistics from the calibration of water quality models in the two estuaries. Example 5.1 gives a visual illustration of how well observations and simulations should agree to help put these statistics into perspective.

From this work by Ambrose and Roesch (1982) and Thomann (1982) it is possible to develop preliminary guidance on how well simulations should agree with measurements to achieve adequate calibration. Ambrose and Roesch (1982) indicate that the coefficient of variation should be 5 to 10 percent for hydrodynamic variables, less than 45 percent for transport variables, and generally less than 90 percent for water quality variables. The correlation coefficient should be greater than 0.94 for hydrodynamic variables, greater than 0.84 for transport variables, and generally greater than 0.60 for water quality variables. The general guidance is summarized in Table 5.15.

Table 5-15. Preliminary Guidance on Error Statistic Criteria for Calibrating Estuarine Water Quality Models

Error Statistics	Criteria for Model Variables				
	Hydrodynamic	Transport	Water Quality	DO	Chlorophyll-a
Relative Error[a]				15%	
Relative Error[b]	±30%	±25%	±45%	±3%	±16%
Cofficient of Variation	10%	45%	90%	17%	70%
Correlation Coefficient	0.94	0.84	0.60	0.80	0.70

[a] See Equation (5.3)
[b] See Equation (5.4)

Example 5.1. Calibration of Hydrodynamics, Mass Transport, and Toxic Chemical Model for the Delaware Estuary

Ambrose (1987) calibrated a tidal transport and volatile chemical model of the Upper Delaware Estuary (see Figure 5.8) to determine if seven volatile chemicals discharged by the Northeast Philadelphia Wastewater Pollution Control Plant (NEWPCP) migrate 6 miles (9.7 km) upstream to the Baxter Drinking Water Plant intake. Earlier versions of the WASP and DYNHYD models (Ambrose et al. 1988) were calibrated using data collected for conventional pollution studies from the summer of 1968 until July 1976, and from volatile chemical data collected in October 1983. The seven chemicals were:

1. Chloroform (CF);
2. 1,2-dichloroethane (DCE);
3. 1,2- dichloropropane (DCP);
4. Dimethoxy methane (DMM);
5. Methylene choloride (MC);
6. Perchloroethylene (PCE), and
7. Trichloroethylene (TCE).

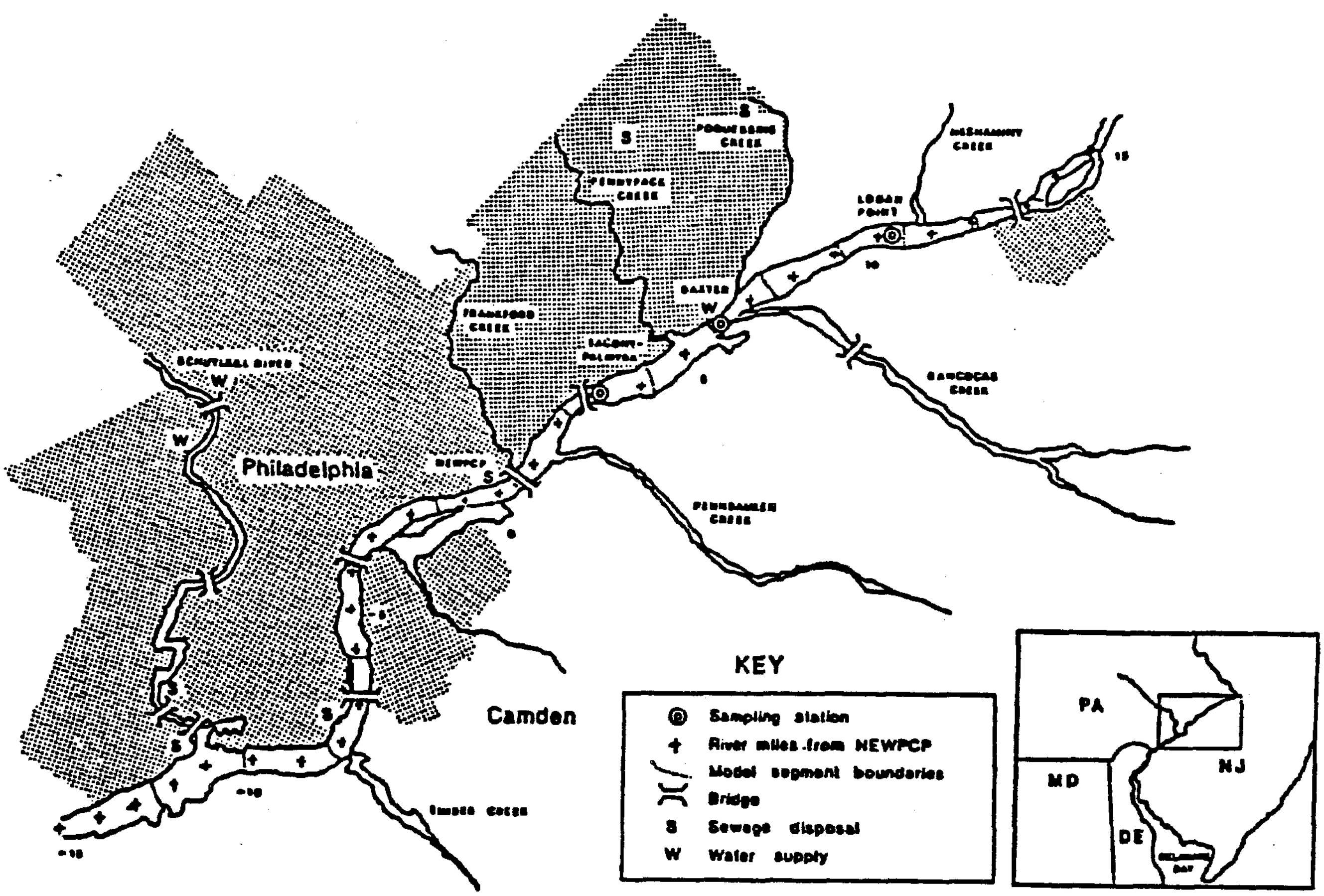


Figure 5-8. Upper Delaware Estuary [Ambrose (1987)].

DYNHYD is a one-dimensional hydrodynamics model that is calibrated by selecting appropriate Manning roughness coefficients and surface drag coefficients. In this case, calibration was based on annual average tidal heights where wind shear was unimportant, leaving only Manning n values to be selected. As noted later in Example 5.4, values of n ranged from 0.020 to 0.045 in various areas of the estuary. Figure 5.9 illustrates the agreement obtained with the selected Manning n values by comparing measured and simulated average spring tide and mean tide (Ambrose 1987). Also see Table 5.7 for a statistical characterization of how well the model was calibrated.

Mass transport components of the model were calibrated using Rhodamine WT dye data collected in July 1974 from a four day steady release from NEWPCP and slack-water salinity measurements. The agreement between simulated and measured slack-water dye concentrations is shown in Figure 5.10. Calibration involved changing the longitudinal dispersion coefficient until the best agreement was obtained. See Table 5.9 for the statistical evaluation of the agreement between measured and simulated characteristics.

The seven problem chemicals were checked and it was found that more that 99% of the total chemical was dissolved in the water column. As a result, suspended sediment parameters were calibrated in an approximate manner using average long term settling, scour and sedimentation data.

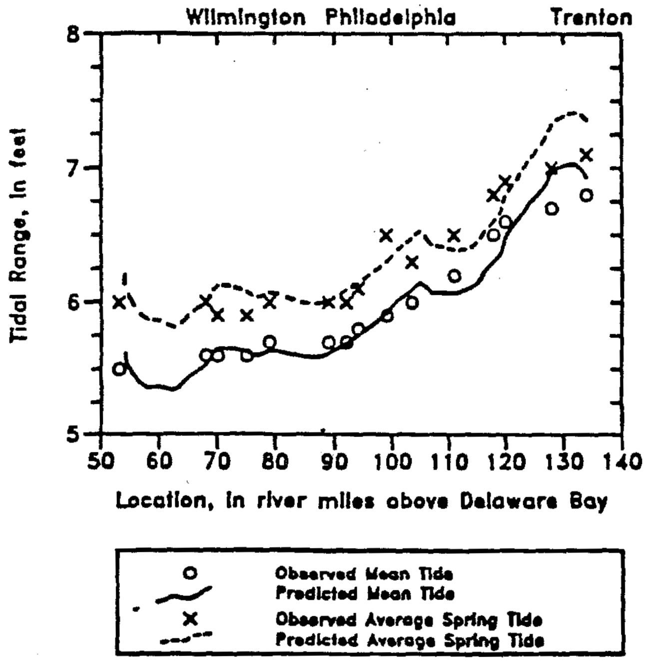


Figure 5-9. Observed and predicted tidal ranges in the Delaware Estuary [Ambrose (1987)].

Chemical rate constants were determined from the literature and by various predictive methods. Volatilization rate constants were determined from the Whitman two layer resistance model using relationships between oxygen, water vapor, and the chemicals of concern. Reaeration was predicted with the O'-Connor-Dobbins (1958) equation (see Supplement XIII). Evaporation was predicted with the regression

Table 5-16. Environmental Properties Affecting Interphase Transport and Transformation Processes [Ambrose (1987)]

Environmental Property	Input Value	Environmental Process K_p[a]	K_s[b]	K_v[c]	K_H[d]	K_o[e]	K_{pH}[f]	K_s[g]
Sediment conc.								
Suspended (mg/L)	20-50	X	X					
Benthic (kg/L)	1.35	X	X					
Organic carbon fraction								
Suspended sediment	0.015	X	X					
Benthic sediment	0.065	X	X					
Sediment settling velocity (m/day)	5.0		X					
Bed sediment resuspension velocity (cm/yr)	5.0		X					
Pore water diffusion (cm^2/s)	1.0×10^{-5}			X				
Benthos mixing factor (0-1)	0.5		X					
Surficial sediment depth (cm)	6.1		X					
Water column depth (m)	3-10		X	X			X	
Water column temp (°C)	25	X	X	X	X	X	X	X
Average water velocity (m/s)	0.65		X					
Wind speed at 10 cm (m/s)	2.0		X					
pH and pOH (standard units)	7.0				X			
Concentration of oxidants (moles/L)	1.0×10^{-9}					X		
Surface light intensity (Langleys/day)	-						X	
Cloud cover (fraction)	0.3						X	
Light extinction coefficient (m^{-1})	3.0						X	
Active bacterial populations								
suspended (cells/ml)	1.0×10^4							X
benthic (cells/100g)	2.0×10^6							

[a] Sorption
[b] Benthos-water column exchange
[c] Volatilization
[d] Hydrolysis
[e] Oxidation
[f] Photolysis
[g] Bacterial degradation

Table 5-17. Chemical Properties Affecting Interphase Transport and Transformation Processes [Ambrose (1987)]

Chemical Properties[a]	Compund Simulated						
	DCP	DMM	DCE	PCE	TCE	MC	CF
General molecular weight (g/mole)	113	76.1	99.0	165.8	131.39	84.94	119.38
Solubility (mg/L)	2.7×10^3	3.35×10^3[b]	8.69×10^3	200	1.1×10^3	2.0×10^4	8.2×10^3
Sorption							
Octanol-water partition, Kow (mg/L octanol per mg/L water)	15	1[c]	30	759	263	18.2	91
Organic carbon partition, K_{OC} (L/kg)	1	0.4	14	364	126	8.8	44
Volatilization							
Henry's Law constant (m^3-atm/mole)	2.31×10^{-3}	1.7×10^{-4}[d]	9.4×10^{-3}	1.53×10^{-2}	9.1×10^{-3}	2.03×10^{-3}	2.88×10^{-3}
Vapor pressure (torr)	2	325[e]	61	14	57.9	362.4	150.5
Volatilization ratio to oxygen	0.53	—	—	0.51	0.55	0.65	0.58
Hydrolysis							
Acid-catalysis rate constant (per molar per hour)	0	0.12[f]	0	0	0	0	0.23
Base-catalysis rate constant (per molar per hour)	0	0	0	0	0	0	0
Neutral rate constant (per hour)	7.2×10^{-4}	0	2.0×10^{-9}	0	0	1.15×10^{-7}	2.5×10^{-9}
Photolysis near surface rate constant (per day)	0	—	0	0	0	0	0
Oxidation constant (per molar per hour)	100	—	100	100	500	100	100
Bacterial degradation second order rate constant (ml per cell per hour)	1.0×10^{-9}	—	1.0×10^{-9}	1.0×10^{-9}	1×10^{-10}	—	—

[a] Values from Mabey et al. (1982) unless otherwise noted [c] Leo et al. (1971) [e] Boublik et al. (1984)
[b] Valvani et at. (1981) [d] Hine and Mookerjee (1975) [f] Shubert and Brownawell (1982)

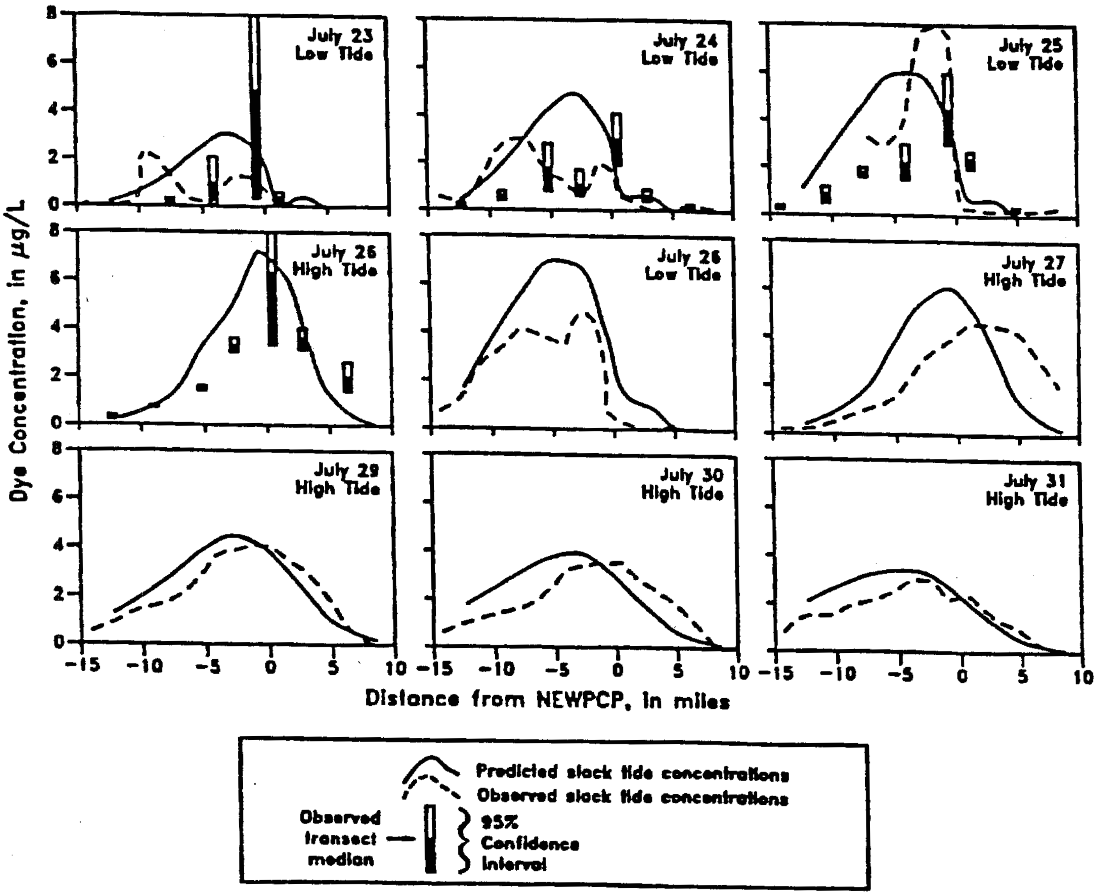


Figure 5-10. Observed and predicted dye concentrations [Ambrose (1987)].

Table 5-18. Predicted Chemical Loss Rate Constants in the Delaware River near Philadelphia [Ambrose (1987)]

Compound Simulated	Predicted Rate Constants (day^{-1})					
	K_V[a]	K_H[b]	K_B[c]	K_O[d]	K_{PH}[e]	K[f]
DCP	0.11	0.02	10^{-4}	10^{-6}	0	0.13
DMM	0.10	10^{-6}	0	–	–	0.10
DCE	0.12	10^{-5}	10^{-4}	10^{-6}	0	0.12
PCE	0.11	0	10^{-4}	10^{-6}	0	0.11
TCE	0.12	0	10^{-5}	10^{-6}	0	0.12
MC	0.14	10^{-6}	–	10^{-6}	0	0.14
CF	0.12	10^{-6}	–	10^{-6}	0	0.12

[a] Volatilization [c] Biodegradation [e] Photolysis
[b] Hydrolysis [d] Oxidation [f] Total

equation of Liss (1973) which ignores the vapor pressure deficit in the atmosphere

$$E = 4.46 + 272.7\,W \tag{5.9}$$

The Evaporation rate is in m day^{-1} and W is wind speed in m sec^{-1} at a 10 cm (0.33 ft) height estimated from 2 m (6.6 ft) measurements in the area and converted to the 10 cm (0.33 ft) height assuming that the logarithmic profile is valid and that the roughness height of the water surface is typically 1 mm (0.0033 ft).

Data defining the environmental properties and chemical properties are reproduced in Tables 5.16 and 5.17. Table 5.18 gives the computed rate constants for volatilization, hydrolysis, biodegradation, oxidation, and photolysis plus the total loss rate constant.

The calibration of the chemical kinetics model is more of a one step validation process of confirming that the literature values are correctly applied for the model and physical conditions at the site. To check the validity of the model, the loads of chemicals and the uncertainty associated with the loads were specified as presented in Figure 5.11. Hydrodynamics and mass transport for the October 1983 period when the volatile chemical samples were collected, were assumed (there were no measurements available) to be governed by mean and spring tides (noted to occur during the study) and a steady freshwater inflow of 3010 ft^3 sec^{-1} (85.2 m^3 sec^{-1}). The model was used to simulate 30 days with mean tide, steady freshwater flow, and constant loads of chemicals from NEWPCP so that a dynamic steady state (i.e., tidal conditions simulated by the model closely matched the simulations of the preceding tidal cycle) was achieved. The simulation was continued one more day to represent the spring tide observed when the volatile chemical samples were collected. These simulations of width and depth average concentrations were compared to the median and range of concentrations obtained from grab samples collected at three locations upstream of the waste inflow. These results are given in Figures 5.12, 5.13, 5.14, and 5.15 for DCP, DMM, DCE, and PCE. The monitoring stations, Tacony-Palmyra, Baxter (water intake), and Logan Point were located at 3, 6, and 11 miles (4.8, 9.7, and 17.7 km) upstream of the waste inflow, respectively. Predicted and simulated concentrations of TCE, CF, and MC were below detection limits (1 μg/L) at the water intake (see Table 5.19).

Table 5-19. Observed and Predicted High Slack Concentrations at Baxter [Ambrose (1987)]

Compound Simulated	Concentrations (g/L) NEWPCP Effluent	Baxter Observed	Baxter Predicted	Error Factor
DCP				
Median	6,050	66	57	1.2^{-1}
95% Interval	1,360-16,800	56-84	12-138	
DMM				
Median	591	9.4	6.2	1.5^{-1}
95% Interval	25-2,820	7.7-13.6	0.3-30	
DCE				
Median	213	2.0	2.1	1.0
95% Interval	67-2,380	1.2-3.0	0.7-24	
PCE				
Median	54	2.1	0.5	4.2^{-1}
95% Interval	30-85	0.2-2.6	0.3-0.8	
TCE				
Median	9.3	0.4	0.09	4.4^{-1}
95% Interval	2.0-33	0-2.5	0-0.3	
CF				
Median	4.4	0.4	0.04	10.0^{-1}
95% Interval	3.2-7.6	0.3-0.9	0.03-0.07	
MC				
Median	2.5	0.04	0.03	1.3^{-1}
95% Interval	1.7-11	0-0.9	0-0.15	

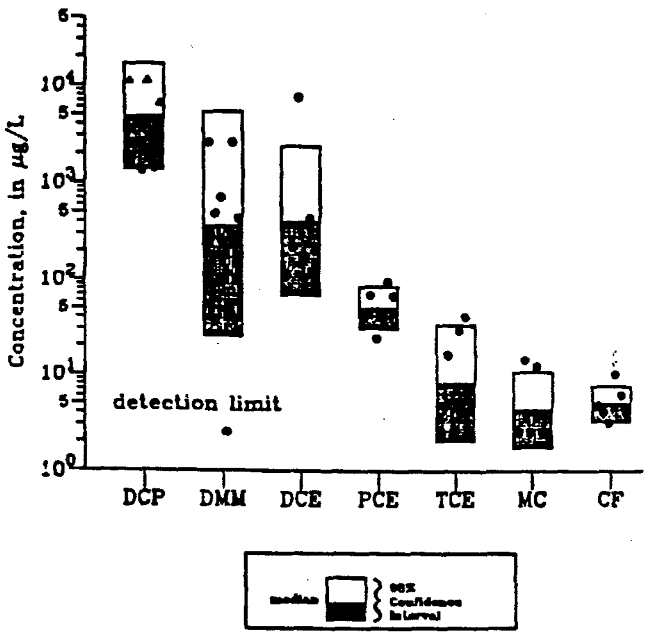


Figure 5-11. Northeast Water Pollution Control Plant Effluent Concentrations, October 2-3, 1983 [Ambrose (1987)].

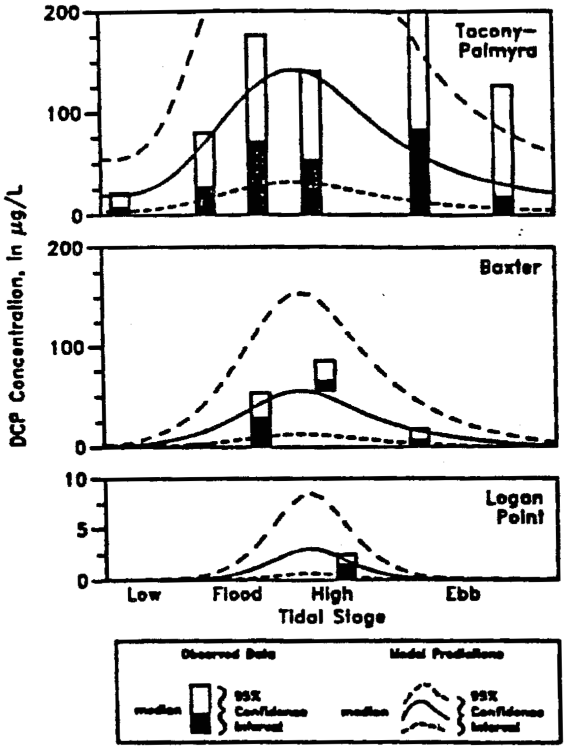


Figure 5-12. Observed and predicted DCP concentrations [Ambrose (1987)].

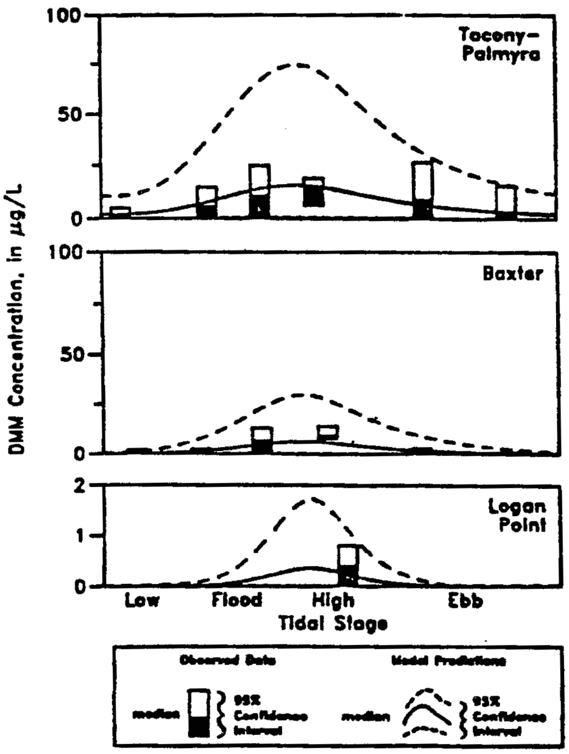


Figure 5-13. Observed and predicted DMM concentrations [Ambrose (1987)].

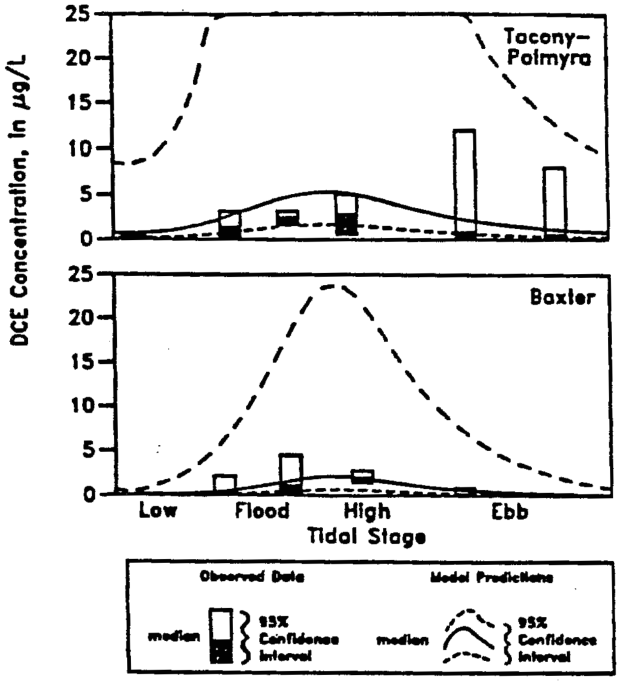


Figure 5-14. Observed and predicted DCE concentrations [Ambrose (1987)].

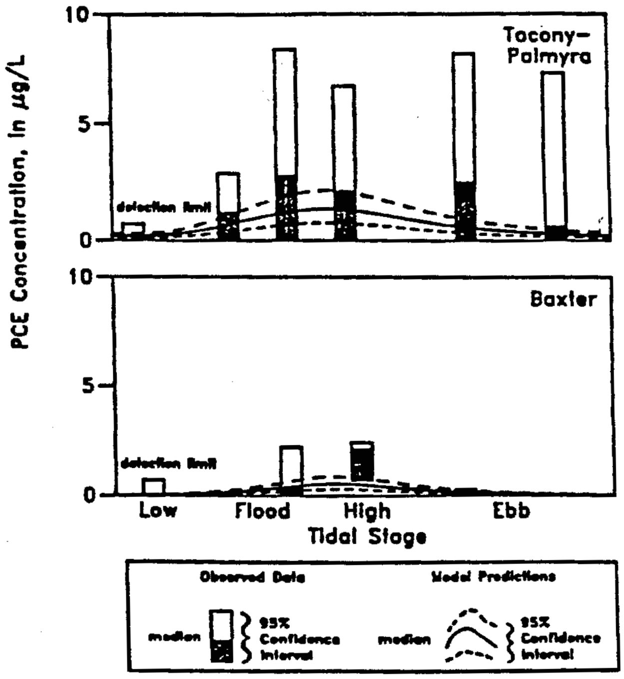


Figure 5-15. Observed and predicted PCE concentrations [Ambrose (1987)].

At this point, the model is sufficiently calibrated to establish a link between the high concentrations measured at the water intake and the waste load and establishes that any other loads are insignificant. Next the concentrations measured at, and predicted at and between monitoring locations can be compared to water quality standards (keeping in mind that this particular model has a tendency to slightly underpredict because of the coefficients chosen from the literature and only predicts averaged values) to determine where water quality standards are violated. If standards do not exist or are not adequate, a human and ecological risk assessment can be performed. If it is determined that the loads should be reduced, the model can be used to make a preliminary estimate of the total load reduction required or after the calibration is refined somewhat to better predict concentrations at the water intake or other critical locations, the model can be used to set loads. To set the final loads, the calibrated model could be used to investigate the effect of extremely low flow and extremely high tides as well as typical conditions.

Jet dilution models can be used to set the mixing zone limits if any are permitted. See Doneker and Jirka (1988) for the recommended model.

5.6 Application Of The Calibrated Model In Waste Load Allocations

Once the model is calibrated and validated, it is then used to investigate causes of existing problems or to simulate future conditions to determine effects of changes in waste loads as part of the waste load allocation procedure. To understand how the calibrated model is used, it is first necessary to review the general waste load allocation procedure.

5.6.1 Waste Load Allocation Procedure

There are several components of the waste load allocation procedure as illustrated in Figure 5.16. The calibration and use of models is only a part of the overall decision making process that also includes some analysis of economic and social issues. Many of the decisions based on economic and social issues have been already addressed in most estuaries and coastal waters but as a general practice, these issues involved in defining water quality standards should be revisited for each study. Also, in local areas of large water bodies some refinement of standards may be necessary, and this should be addressed as part of a general procedure. Typically, the regulatory agency

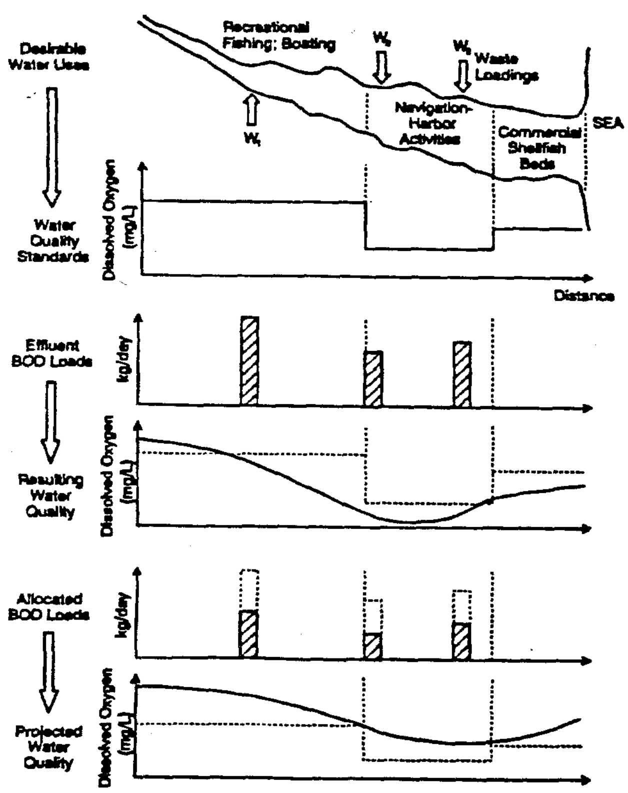


Figure 5-16. Componennts of the waste load allocation procedure.

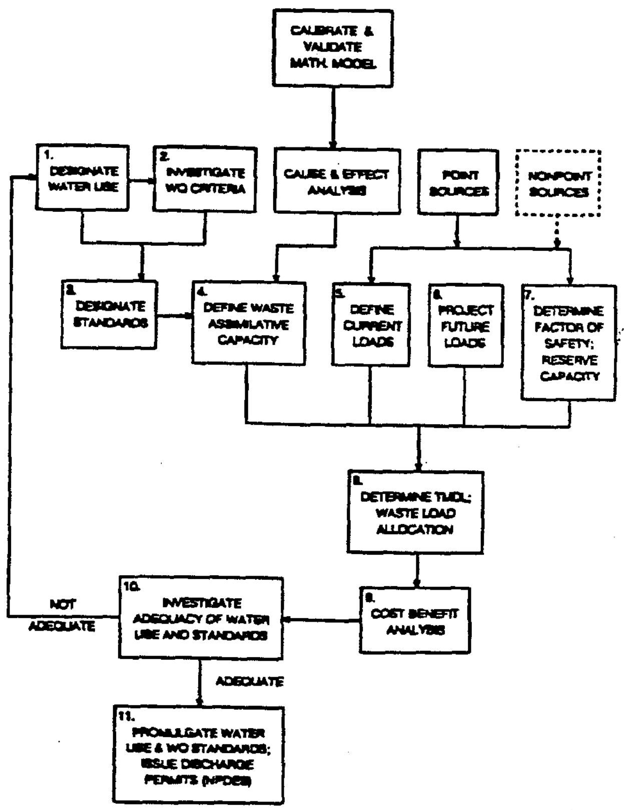


Figure 5-17. General waste load allocation procedure. Note WQ = water quality, NPDES = National Pollution Discharge Elimination System, and TMDL = total maximum daily load.

Table 5-20. Main Sources of Criteria to Protect Designated Water Uses

Primary Documents	EPA's "Gold Book" - US EPA, Quality Criteria for Water 1986 (with updates), Rept. EPA 440/5-86-001, Office of Water Regulations and Standards, Washington, D.C., U.S. Government Printing Office, No. 995-002-00000-8. Any State criteria documents for the water body of interest.
Secondary Documents	Any information available in the open literature.
Historical Documents*	EPA's "Red Book" - US EPA, Quality Criteria for Water, Rept. EPA 440/5-86-001, Washington D.C. (superseded by EPAS's "Blue Book" - Environmental Studies Board, National Academy of Sciences and National Academy of Engineering, Washington, D.C., Rept. EPA-R3-73-033, 1973). "Green Book" - Report of the Committe on Water Quality Criteria, Federal Water Pollution Control Administration, U.S. Department of the Interior, Washington, D.C. 1968. McKee, J.E., and wolf, H.W., Water Quality Criteria, 2nd edition, California State Water Quality Control Board, Sacramento, 1963. Water Quality Criteria, California State Water Quality Control Board, Sacramento, 1952. See p. iii of the Red Book for pre-1950 work in this area.

* Useful for tracing the development of criteria and citation of additional information

should determine that the published standards are still valid and useful.

The general procedure for waste load allocation is shown in Figure 5.17 and has the following steps (Thomann and Mueller 1987, Krenkel and Novotny 1980, Driscoll et al. 1983):

1. Designate desirable water uses for the estuary, coastal area, or harbor of interest. Examples include maintaining water quality to permit commercial fin and shell fishing, maintain habitat diversity to protect the ecological health of the estuary, to allow use of the water in industrial applications such as process cooling, use of water for drinking in freshwater segments, recreational boating and fishing, and use of the estuary for navigation.

2. Investigate criteria available to protect the desired water uses. See Table 5.20 for the main criteria documents.

3. Select numerical criteria to protect the designated uses (i.e., 5 mg/L dissolved oxygen to protect certain fish species).

4. Define waste assimilative capacity. This involves the use of a water quality model or simplified analysis to determine the cause and effect relationship between existing and projected loads, and water quality response of the estuary. The modeling alternative involves calibration and validation of the model with site-specific data as described in this section. The simplified analysis (see Mills et al. 1985) involves analysis of existing data and some engineering judgement (typically from experts). The complexity of estuary problems usually overwhelmingly favors a modeling approach.

5. Define existing loads. This is done as part of the calibration of any model used to determine the assimilative capacity but these load measurements may not provide all the information required. In addition, the typical loads and maximum loads must be determined for any sensitivity analysis and projection of critical effects. When the analysis focuses on point sources (i.e., when nonpoint sources are unimportant), the study is termed *Waste Load Allocation*. When the analysis focuses on nonpoint sources, the study is termed a *Load Allocation*. *Total Maximum Daily Loads* are determined from both the Waste Load Allocation and Load Allocation. The definition of existing and projected loads are usually best done in cooperation with the discharger when strict quality assurance of the data is possible.

6. Project future loads. This step defines future capacity required for continued economic growth in an area and is done in consultation with the industries and municipalities involved.

7. Determine a factor of safety or reserve capacity. This is largely a policy matter involving what degree of protection will be afforded. This should account for uncertainty in the calibrated model and projection of future loading.

8. Determine Total Maximum Daily Loads and individual dischargers waste load allocations (see EPA 1985 for definitions). This includes simulation with existing and projected loads, and incorporation of reserve capacity to determine what load reductions or projected loads will allow the water quality to remain at or above the standards chosen. Decisions on how to allocate load reductions to various dischargers depends on the weighting scheme chosen by each state agency and is typically based on state law and regulation. The decision should be influenced by economic and social factors that encompass differences in the ability of municipalities and industries to

and industries to achieve load reductions (i.e., differences in economic efficiency). Equity should also be considered to account for past efforts to voluntarily reduce loads and to account for differences between the dischargers who have been located on the estuary for different lengths of time. A sensitivity analysis, first order error analysis, and Monte Carlo analysis is used to determine the uncertainty in the total maximum daily loads selected. See Brown and Barnwell (1987) for examples of how uncertainty analysis is applied to streams.

9. For the total maximum daily loads selected, evaluate the cost-benefit of the standards chosen. This step may be somewhat controversial and applied in different ways. In general, however, the analysis should consider:

   a. Individual costs to the dischargers

   b. Regional costs and the associated benefits of improved water quality.

   In practice it may difficult to separate steps 8 and 9 of the procedure.

10. If the economic analysis is favorable, the full effects on present and future water quality are examined. If appropriate, standards may be upgraded if necessary to prevent degradation of existing water quality (Krenkel and Novotny 1980). If meeting the standards represents a significant economic or social impact, adoption of different standards to forgo some water uses may be in order.

11. If the standards and waste load allocations are adequate, the standards are promulgated and the NPDES (National Pollution Discharge Elimination System) permits are issued.

5.6.2 Critical Water Quality Conditions and Projections

Once critical water quality conditions are defined for the estuary, harbor or coastal area of concern, determining the waste assimilative capacity is relatively straightforward. Models are available to relate critical water quality responses to the loads for most problems. See Chapter 3 for guidance.

However, the definition of critical conditions for estuaries is not straightforward. For streams receiving organic loads, this is a straightforward matter of determining the low flow and high temperature conditions. In estuaries, fresh water, tides, wind, complex sediment transport, and other factors can be important to determining the critical conditions. As of yet, there are no clear methods to establish critical conditions, especially in terms of the probability of occurrence. The analyst must use considerable judgement in understanding the exact effects of the processes described in Chapter 2.

Once loads are set or if critical conditions or future conditions are to be simulated, the calibrated model can be used to predict the response to the different conditions. The investigation may involve study of extreme hydrological, meteorological, or hydrographic events that affect mixing; waste loadings from point and non-point sources; and changes in benthic demands. If the physical, chemical, and biological characteristics of the estuary or wastes entering the estuary are changed, then it may be necessary to modify model coefficients. However, these changes can not be reliably predicted. As a result, some sensitivity analysis is necessary to assist in selection of the appropriate safety factor in the total maximum daily load.

Extreme circulation events can move sludge deposits out of the estuary or into the estuary. Point source reduction can cut off the organic deposits that cause SOD. Nevertheless, it is not presently possible to make more that crude estimates of the reduced SOD. Greater degrees of waste treatment can also reduce deoxygenation coefficients but it is not clear why this occurs and when it should be expected. As a result, estimates of the effects of changes in SOD, the deoxygenation coefficient, and other parameters are routinely made to see if a significant effect can occur, but final calculations may conservatively assume that the rates remain unchanged.

Occasionally, estimates of the effects on SOD can be made by experts such as those with EPA Region IV who have made extensive measurements in polluted and clean areas and who understand how to conservatively extrapolate to future conditions. In addition, it is possible to consult the existing data and make reasonable estimates. See Supplement XV for guidance. Crude estimates of deoxygenation rate coefficients can also be made in a similar manner but with less certainty. Tabulations of deoxygenation coefficients for different types of conditions may be less certain because of the errors of calibration contained in the tabulated estimates. Nevertheless, when some judgement is employed, the tabulations and guidance given in Supplement IX is usually adequate.

5.6.3 Component Analysis and Superposition

Applications involving setting total maximum daily loads and individual waste load allocations for dissolved oxygen problems are conceptually simplified in many cases by noting that a linear relationship usually exists between loads and deficits. Only when phytoplankton and second order toxic chemical modeling is required, does a nonlinear relationship between deficits or chemical concentrations and load exist. It is also possible to investigate which components of a waste load (unoxidized carbon or nitrogen versus nutrients that result in eutrophication), cause a dissolved oxygen deficit. The linear relationship between waste load components and deficit or other chemical concentrations (e.g., BOD or ammonia) is also very useful to investigate the effect of multiple sources. A component analysis can be performed to determine the effect of each load. For additional information, see Thomann and Mueller (1987), Krenkel and Novotny (1980), and Mills et al. (1985).

Investigation of existing problems is best pursued with a components analysis that indicates those processes and loads that contribute to the problems. For example, the cause of violations of a dissolved oxygen standard can be determined from the relative contribution of various loads and the effect of sediment oxygen demand, BOD decay, nitrification, photosynthesis, and reaeration. This is illustrated in Example 5.2 from Robert Thomann in review. Components of the maximum deficit are computed by keeping up with the deficit calculated in each time step for each process: reaeration, deoxygenation, nitrification, sediment oxygen demand, net photosynthesis, and by dilution with other loads and tributaries.

Multiple sources that do not significantly increase estuary flow are usually handled in an additive fashion according to the principle of superposition (Thomann and Mueller 1987, Krenkel and Novotny 1980, and Mills et al. 1985) as indicated above, since all water quality models are linear except for phytoplankton kinetics and when toxic chemical kinetics are not first order. Therefore, a component analysis like that in Example 5.2 would be performed that would separate individual loads and the analysis would determine which loads cause the maximum deficit or any deficit below standards. Where different point sources contribute to one problem, some arbitrary allocation of more restrictive treatment requirements based on state policy will be necessary as discussed above. The superposition of multiple sources is illustrated in Examples IV-3, IV-5, IV-6, and IV-8 from Mills et al. (1985).

Example 5.2 Component Analysis of Dissolved Oxygen Balance in the Wicomico Estuary, Maryland

The Wicomico Estuary is a small arm of Chesapeake Bay. Figure 5.18 shows the location of the Salisbury Sewage Treatment Plant outfall, other tributaries, and the model segmentation of the estuary. The problem is to determine the required additional treatment beyond secondary levels at the Salisbury, Maryland Sewage Treatment Plant (Robert Thomann, in review). To perform the analysis, a one-dimensional model was calibrated for the estuary and a component analysis of the dissolved oxygen balance was performed along the axis of the estuary. The results are given in Figure 5.19. The upper panel gives the dissolved oxygen deficit along the estuary where a maximum deficit of almost 4 mg/L occurs near Mile 10 (km 16) down estuary of the outfall. Near the outfall, the estuary is supersaturated with oxygen. The component analysis in the lower three panels shows that the discharge of carbonaceous and nitrogenous demands from the sewage treatment plant and the upstream deficit do not contribute to the maximum deficit. However, the discharge of excess nutrients was a problem. The growth of phytoplankton due to chlorophyll *a* levels of 300 ug/L was stimulated by nutrients in the waste discharge. The management decision for this waste load was then to control the level of nutrients rather than increase the level of carbon or nitrogen treatment (Robert Thomann in review).

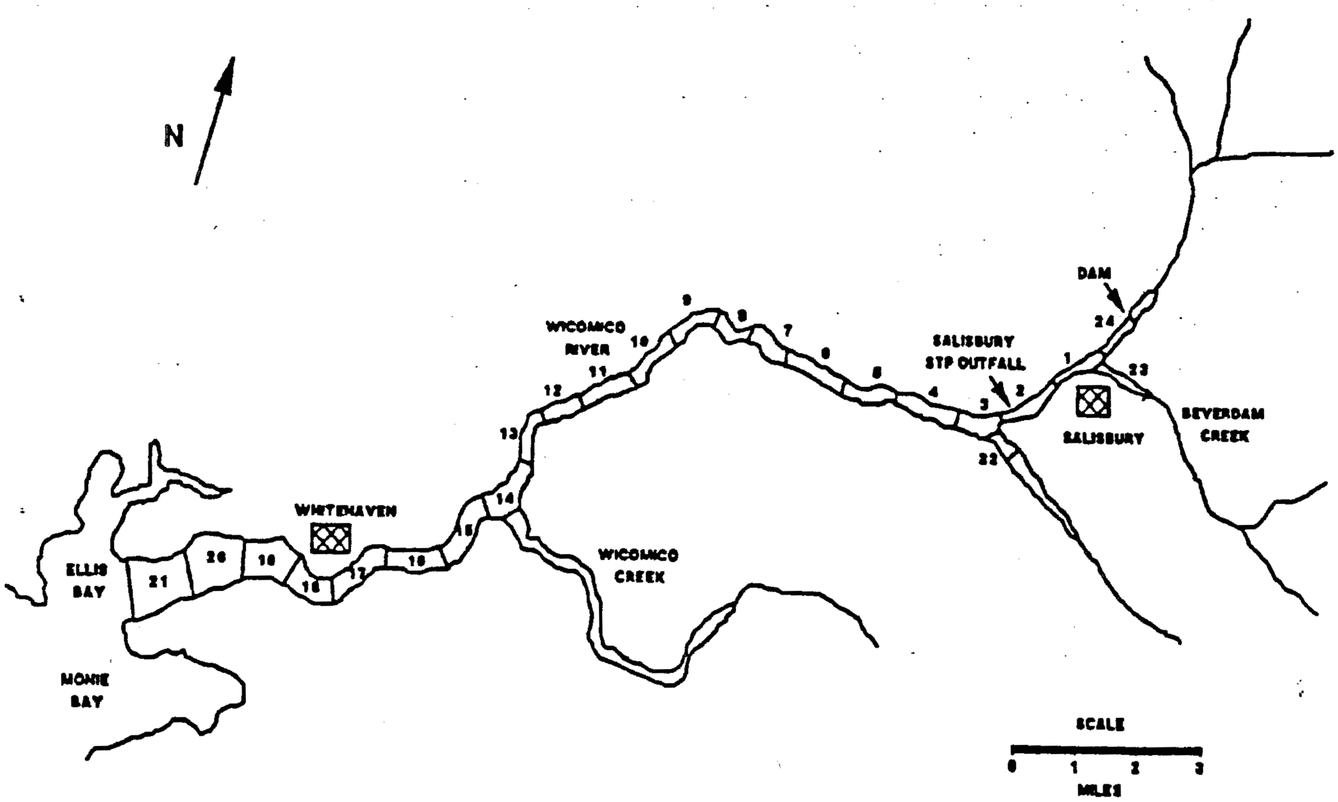


Figure 5-18 Model segmentation - Wicomico River, Maryland.

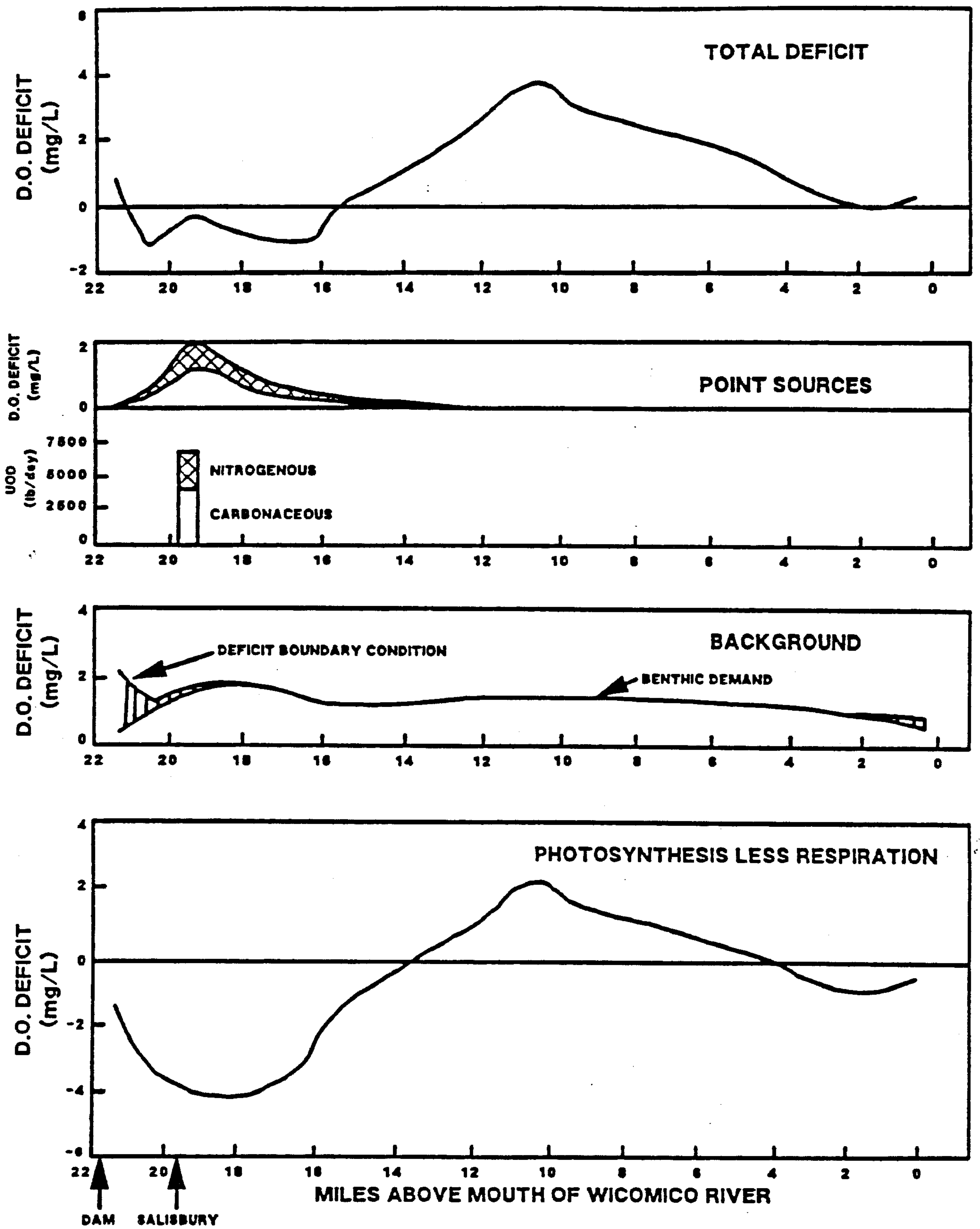


Figure 5-19. Component deficits for July 1971 dissolved oxygen verification [Robert Thomann in Review].

SUPPLEMENT I: SELECTION OF MANNING n VALUES

The effect of bottom friction on the flow in estuaries is represented in a variety of ways in flow or hydrodynamic models. The most common method used in the United States and in many other countries, employs the Manning roughness coefficient to quantify friction and turbulent hydraulic losses in the flow. However, a number of other friction coefficients are used in the models available. These are given in Table 5.21 along with the relationship between coefficients.

In models with vertical resolution (i.e., having more than one layer), the Manning n is used to compute stress at the bottom boundary in a series of relationships between n, the drag coefficient (C_d), and turbulent mixing. The quadratic stress formulation relates the eddy viscosity approximation of the vertical Reynolds stress to a drag coefficient and average velocities as follows

$$\rho_o E_z\,(\partial u/\partial z) = \rho_o C_d\,(u_b{}^2 + v_b{}^2)^{0.5}\,(u_b) \qquad (5.10)$$

and

$$\rho_o E_z\,(\partial v/\partial z) = \rho_o C_d\,(u_b{}^2 + v_b{}^2)^{0.5}\,(v_b) \qquad (5.11)$$

where

ρ_o = density of water,

$\partial u/\partial z$, $\partial v/\partial z$ = the vertical velocity gradient in the x and y directions, respectively,

u_b, v_b = horizontal velocities at a point above the bottom in the x and y directions, respectively, and

E_z = vertical eddy viscosity.

The drag coefficient is related to the Manning n as shown in Table 5.21

$$C_d = \frac{g n^2}{C_1{}^2 R_H{}^{1/3}} \qquad (5.12)$$

Also any other friction factor or roughness coefficient can be used from Table 5.21. Equations (5.10 and 5.11) represent terms in the conservation of momentum equations given in Table 2.1 of the second section in Part I of this guidance manual. The two- and three-dimensional models based on these formulas are calibrated by varying the Manning n until any measurements of average velocity and tidal amplitude at a number of sites plus any observations of salinity intrusion are properly described by the model. When models discretization elements are reduced to smaller and smaller scales, the calibration values of the Manning n approach values only controlled by the scale of roughness on the bottom. In the limiting case where the bed is flat, the Manning n can be estimated for sand

Table 5-21. Relationship between Various Friction Factors used to Quantify Friction Loss in Estuaries

	Manning n	Chezy C_z	Drag Coefficient $C_d = u^{*2}/U^2$	Darcy-Weisbach f	Fanning f_f
Manning n	$= n$	$= \frac{C_1}{C_z} R_H{}^{1/6}$	$= \frac{C_d^{1/2} C_1 R^{1/6}}{g^{1/2}}$	$= \frac{C_1 R_H{}^{1/6} f^{1/2}}{(8g)^{1/2}}$	$= \frac{C_1 R_H{}^{1/6} f_f{}^{1/2}}{(2g)^{1/2}}$
Chezy Cz	$= \frac{C_1}{n} R_H{}^{1/6}$	$= C_z$	$= \frac{g^{1/2}}{C_{d1}^{1/2}}$	$= \frac{(8g)^{1/2}}{(f)^{1/2}}$	$= \frac{(2g)^{1/2}}{(f_f)^{1/2}}$
Drag Coefficient Cd	$= \frac{g n^2}{C_1^2 R^{1/3}}$	$= \frac{g}{C_z{}^2}$	$= C_d$	$= \frac{f}{8}$	$= \frac{f_f}{2}$
Darcy-Weisbach f	$= \frac{8 g n^2}{C_1^2 R^{1/3}}$	$= \frac{8g}{C_z{}^2}$	$= 8 C_d$	$= f$	$= 4 f_f$
Fanning f_f	$= \frac{2 g n^2}{C_1^2 R^{1/3}}$	$= \frac{2g}{C_z{}^2}$	$= 2 C_d$	$= \frac{f}{4}$	$= f_f$

Notes:

1) C1 = unit conversion factos; equal to 1.0 if the hydraulic radius R is expressed in units of meters and 1.49 if expressed in units of feet.
2) The Fanning friction factor is typically used in mechanical engineering applications.
3) Reports of values of the drag coefficient should be accompanied by a definition of Cd. Alternatively, Cd has been defined [Chow (1959), Streeter and Wylie (1975)] as $\tau_0 = (1/2)\rho\, C_d U^2$ or $C_d = 2u_*{}^2/U^2$ where bed shear velocity, τ, divided by water density, ρ, is the shear velocity, $u_* = (g R_H S)^{1/2}$. S is the energy gradient of the flow. U is the average flow velocity.

and gravel beds using an approximate form of Sticklers equation (Henderson 1966, Garde and Ranga Raju 1977)

$$n_b = 0.031\, d^{1/6} \quad (5.13)$$

where d is the diameter in feet of bed sediments that are larger than 75 percent of the material present. If the diameter, d, is expressed in meters

$$n_b = 0.025\, d^{1/6} \quad (5.14)$$

These expressions for n_b should be valid for many estuarine flows where rough turbulent flow is expected to be the predominate flow regime. In general, however, flow resistance is a function of the Reynolds number of the flow

$$\mathrm{Re} = \frac{4UR}{\nu} \quad (5.15)$$

where U is the average flow velocity, R is the hydraulic radius (cross sectional area divided by wetted perimeter), and ν is the kinematic viscosity of estuarine waters. Figure 5.20, modified from a Moody diagram for flow resistance, gives the general relationship between the ratio of the Manning n to depth to the one-sixth power (hydraulic radius is approximately equal to depth in wide water bodies) and Reynolds number. The curves for sand-coated surfaces should be used to estimate n_b for estuaries when sandy bottoms are observed.

The smooth surface curve shown in Figure 5.20 may be approached when fluid mud layers are observed on the bottom. Typically, fluid mud may occur near or just downestuary of the turbidity maximum where significant deposition is expected. For example, values of n were found to be approximately 0.018 to 0.020 near the turbidity maximum in the Delaware Estuary (Ambrose, personal communication, Ambrose 1987, Ambrose and Roesch 1982, Thatcher and Harleman 1981). Occasionally, unrealistically low values of n (i.e., n = 0.015) normally associated with very smooth surfaces may be indicated by calibration. These values may not be consistent with Figure 5.20. The reason is that stratification of the flow near the bed by fluid mud or suspended sediment significantly decreases the apparent roughness coefficient (McCutcheon 1979, 1981, McDowell and O'Connor 1977). Where this occurs, the calibrated hydrodynamics model can be expected to have an extremely limited range of applicability since the fine scale effects of sediment stratification are not incorporated into vertically averaged models or models having gross repre-

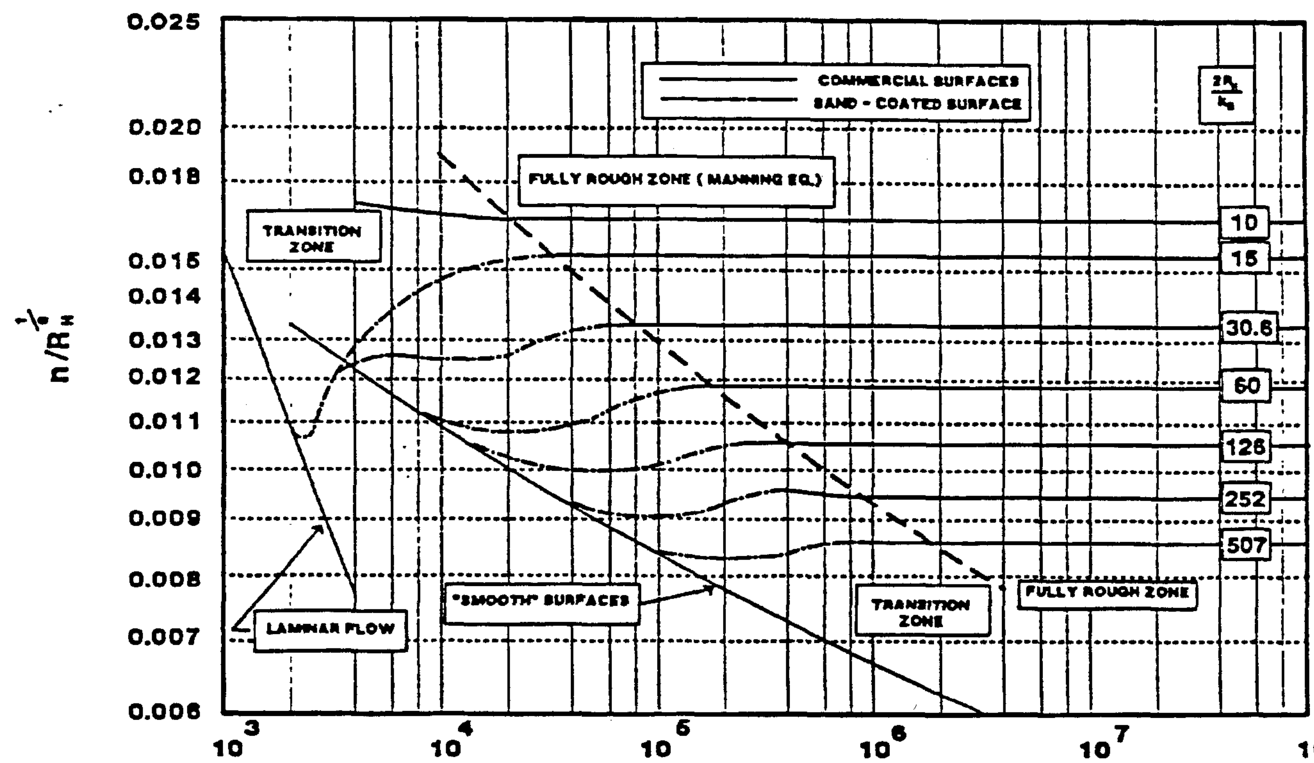


Figure 5-20. Modified moody diagram relating the Manning n to Reynolds number. k_s is sand grain height and R_H is the hydraulic radius.

Table 5-22. Values of the Manning n for Different Types of Vegetation in Wetland Areas [Chow (1959) and Jarrett (1985)]

Type of Vegetation	Value of n		
	Minimum	Typical	Maximum
Grass:			
Short	0.025	0.030	0.035
Tall	0.030	0.035	0.050
Brush:			
Scattered with Dense Weeds	0.035	0.050	0.070
Sparse Trees and Brush in Winter	0.035	0.050	0.060
Sparse Trees and Brush in Summer	0.040	0.060	0.080
Medium to Dense Brush in Winter	0.045	0.070	0.110
Medium to Dense Brush in Summer	0.070	0.100	0.160
Trees:			
Dense, Straight Willows	0.110	0.150	0.200
Stumps or Cyprus Knees	0.030	0.040	0.050
Stumps with Dense Sprouts, Grass and Weeds	0.050	0.060	0.080
Dense Stand of Trees, Few Fallen Trees, and no Branches hanging in water	0.080	0.100	0.120
Dense Stand of Trees, Some Fallen Trees, or Branches Hanging in Water	0.100	0.120	0.160

sentation of the vertical structure. When this occurs, it is important to conduct a sensitivity analysis to determine if the overall calibrated model shows any sensitivity in the important decision variables (i.e., dissolved oxygen, chlorophyll a, or sedimentary contaminant concentrations, etc.) to values of n.

There are also effects of vegetation on flow in shallow parts of estuaries that may need to be taken into account, especially if the trend to employ natural or created wetlands to aid wastewater treatment continues. First, sea grass and other vegetation influence shallow open water flows. Second, emergent vegetation such as cyprus trees, mangroves, bushes, and marsh grasses may control flow through wetland areas. At present, there do not seem to be many studies of the effect of sea grass on friction loss (personal communication, Florida Dept. of Environmental Regulation, 1989). There are, however, investigations of friction losses in grassed open channels that show that losses are a complex function of the Reynolds number. As flow increases, grasses are pushed flatter along the bottom and less area of grass is in direct contact with the flow. In effect, the relative roughness decreases as a function of flow velocity or Reynolds number. Perhaps the best study of this effect is by Chen and the US Geological Survey.

In the absence of solid guidance on this topic, it should be noted that Chow (1959), Jarrett (1985) and others give guidance on the effect of grass on channel and overbank flow. Values on the order of 0.025 to 0.050 are reasonable.

In wetlands and other areas of emergent vegetation, relative roughness is less likely to vary and the Manning n is expected to be constant. The scale of the roughness is considered to be the trunk diameter that should not change significantly as depth increases. Values have not been well defined, but values of river flow over flood plains is very applicable when the density and trunk size of the vegetation are similar. Values as high as 0.20 have been observed, as noted in Table 5.22.

In addition to the older information in Table 5.22, Arcement and Schneider (1984) report more recent information for more tranquil flows in floodplains. However, it is not expected that n can be precisely defined in any published study. Flow in wetlands occurs in ill defined channels where the uncertainty in average velocity, area, depth, and slope make it very difficult to determine n.

As larger and larger model scales are employed, more and more large scale turbulent friction losses due to flow non-uniformity must be included in estimates of the Manning n to adequately represent losses due to energy dissipation. Empirical relationships have not been derived for this purpose but similar corrections of this nature have been derived for river flows that can be used as guidance. Guidance for riverine reaches works well in the upper sections of estuaries where the transition from riverine conditions occur. The guidance is less useful downestuary where the scales of flow may increase by an order of magnitude in some cases.

Conceptually, the riverine estimation procedure can be formulated as a process of modifying a base value of the Manning n such that

$$n_{composite} = n_b + n_f + n_1 + n_2 + n_3 \qquad (5.16)$$

where typical values are on the order of 0.020,

n_b = Manning n associated with bottom roughness conditions,

n_f = correction related to form roughness or bed irregularity due to ripples and dunes,

n_1 = correction related to the nonuniform depth of the flow, and

Table 5-23. Manning n Corrections for Ripples and Dunes

Bed Topography	n_f
Smooth Bed	0.00
Ripples	0.005
Dunes	0.010

Table 5-24. Manning n Corrections for the Relative Effect of Obstructions

Relative Effect of Obstructions	n_1
Negligible	0.00
Minor	0.010 to 0.015
Appreciable	0.020 to 0.030
Severe	0.040 to 0.060

Table 5-25. Manning n Corrections for Changes in Channel Depth and Width

Variation of Channel Cross Section	n_2
Gradual	0.00
Alternating occasionally	0.005
Alternating frequently	0.010 to 0.015

n_2 = correction for the nonuniform width of the flow.

n_3 = correction for effects of vegetation

Alternatively, Chow (1959) notes that a multiplicative version of Equation (5.16) can be used as well. However, that form is better adopted to meandering channels and is not very suitable for estimates in estuaries.

Values of n_f are approximately 0.00 to 0.010 (Chow 1959) as shown in Table 5.23. Values of n_1 and n_2 can be estimated approximately from the effect of obstructions and channel cross section variations given by Chow (1959) in Tables 5.24 and 5.25. Table 5.26 gives corrections for the effect of vegetation. It should be noted however, that these constant corrections may not be adequate since the correction for seagrasses and kelp probably vary with flow velocity or Reynolds number.

In models that assume that the flow field can be vertically and laterally averaged, the one-dimensional equations of motion and continuity can be written as (Thatcher and Harleman 1981, Ambrose et al. 1988)

$$\frac{\partial Q}{\partial t} = -\partial\frac{(QU)}{\partial x} - gA\frac{\partial h}{\partial x}\frac{gn^2Q\,|Q|}{AC_1{}^2R_H{}^{4/3}}$$

$$-g\frac{Ad_c}{\rho}\frac{\partial\rho}{\partial x} + \frac{AC_{da}\rho_a}{R_H\rho}W_{10}{}^2\cos\alpha \qquad (5.17)$$

and

Table 5-26. Adjustments for the Manning n due to Vegetation [Jarret (1985)]*

Amount of Vegetation	Range of n_3	Description of Conditions
Small	0.002 to 0.01	Dense growths of grass or weeds, average depth at least twice the height of grass, or supple seedlings where the flow is at three times the height of the vegetation.
Medium	0.010 to 0.025	Grass from 1/2 to 1/3 of the depth; moderately dense large stem grass, weeds, or tree seedlings 1/2 to 1/3 the depth of flow; or moderately dense bushy trees like 1 to 2 year old willows.
Large	0.025 to 0.050	Grass over the full depth of flow; 8 to 10 year old trees with some brush and weeds; or 1 year old trees with heavy weeds and foliage.
Very Large	0.050 to 0.100	Flow depth half the height of dense grass; bushy willow trees with dense weeds, grass and foliage; dense cattails; or trees with heavy undergrowth and full foliage.

$$b\frac{\partial h}{\partial t} + \frac{\partial Q}{\partial x} - q = 0 \qquad (5.18)$$

where

$\frac{\partial Q}{\partial t}$ = local inertia term,

$\partial\frac{(QU)}{\partial x}$ = force due to advection or momentum change due to mass transport of water,

$gA\frac{\partial h}{\partial x}$ = force due to potential energy of the fluid or gravitational body force,

$\frac{gn^2Q\,|Q|}{AC_1{}^2R_H{}^{4/3}}$ = force due to bottom shear or frictional resistance (quadratic stress law),

$g\frac{Ad_c}{\rho}\frac{\partial\rho}{\partial x}$ = force due to longitudinal pressure difference caused by density differences along the axis of the estuary,

$\frac{AC_{da}\rho_a}{R_H\rho}W_{10}{}^2\cos\alpha$ = Force due to wind shear on the water surface,

Q = Discharge (Q = UA),

U = Longitudinal velocity averaged over the cross section and averaged over time,

t = time,

x = Longitudinal direction along the axis of the estuary,

g = Gravitational constant,

A = Cross sectional area,

$\frac{\partial h}{\partial x}$ = Slope of the energy gradient or approximately the water surface slope, where h is the depth of flow to water surface from an arbitary datum,

n = Manning roughness coefficient,

C_1 = Units conversion factor (1.0 when R_H is expressed in m and 1.49 when R_H is expressed in feet),

R_H = Hydraulic radius (cross-sectional area divided by wetted perimeter of the cross section that is approximately equal the depth in wide estuaries),

d_c = Distance from water surface to the centroid of the cross-section,

C_{da} = Drag coefficient for air moving over water surface (typically assumed constant and having a value of 0.0025 or slightly less),

ρ_a = The density of air,

ρ = Density of water,

α = Angle of wind direction from the axis of the estuary,

W_{10} = Wind speed measured at 10 above the water surface,

b = Total surface width, and

q = Lateral inflow per unit length.

Equations (5.17) and (5.18) are accurate approximations when lateral and vertical differences are unimportant, which is the case in many estuaries. However, a more approximate equation has proven almost as widely applicable. The approximation is the link-node model that assumes that the one-dimensional estuary can be divided into a series of uniform channels between nodes. The cross section may vary from one channel to the next and any flows into the estuary are assumed to enter at the nodes. It is also assumed that longitudinal pressure differences due to pressure gradients are small enough to neglect. The best examples of link-node models are the EXPLORE I (Baca et al. 1973), DEM (Dynamic Estuary Model) (Feigner and Harris 1970), and the derivations of these models such as the DYNHYD model used with the WASP modeling package (Ambrose et al. 1988). The approximate equations are written as

$$\frac{\partial U}{\partial t} = -U\frac{\partial U}{\partial x} - g\frac{\partial h}{\partial x} - \frac{g n^2}{C_1{}^2 R_H{}^{4/3}} U\ |U|$$

$$+ \frac{C_{da}}{R_H}\frac{\rho_a}{\rho} W_{10}{}^2 \cos\alpha \qquad (5.19)$$

and

$$\frac{\partial A}{\partial t} = \frac{-\partial Q}{\partial x} \qquad (5.20)$$

Since Equations (5.19) and (5.20) have been used extensively, some care may be necessary to interpret results relating to selections of the Manning n. Any effects of neglecting longitudinal, vertical, and lateral salinity gradients and accelerations due to nonuniform channels will be lumped into the value of the roughness coefficient used to calibrate the model. Normally, these effects are minor and relatively reliable guidance can be formulated.

Guidance on the selection of Manning n values is as follows:

1. **Select initial values based on bed material and correct for bed variations** - Values should be uniform for areas where bottom topography, channel alignment and sediment size distributions do not vary significantly. Smaller values should be selected for bottoms covered with fluid mud or other fine-grain material. Typically a value of 0.02 is appropriate for reaches with fine grain sediments and 0.025 to 0.030 is appropriate for reaches with sand bottoms. If necessary, a precise initial estimate can be made by computing the Reynolds number and the relative roughness (i.e., $2R/k_s$, where k_s is the sand grain diameter or the height of the ripples and dunes) and consulting Figure 5.18. If the bed is covered with vegetation (i.e., none of the sediments are in contact with the flow) then Table 5.22 should be used to select an n value and correct for variations in cross section, bottom topography, and obstructions. If the bed is partially covered with vegetation, the initial selection should be based on the bed materials present and corrections should be made for vegetation, and variations in cross section, bottom topography, and obstructions. Where it is not clear whether exposed bed materials are important in causing friction losses, both procedures should be followed to see if any significant discrepancies exist.

2. **Correct for bed roughness** - Table 5.23 shows the corrections that should be added if bed ripples and dunes are present on the bed. A correction should not be made if Figure 5.20 is used and the roughness height is assumed to be the height of ripples and dunes.

3. **Correct for topographic variability** - Values may need to be increased in computational elements or reaches in which there is a significant change in bottom elevation or where channels narrow. Increased n values are required to compensate for friction loss due to non-uniform flow conditions. Tabulated values of the Manning n (Chow 1959, French 1985, Henderson 1966, Barnes 1967) do not reflect the increased turbulence due to non-uniform flow. It should be noted that these corrections can only be approximated because friction losses in nonuniform flows are dependent on flow direction. Losses are significantly greater when the flow speeds up and contracts into a shallower or narrower channel compared to expansion into a deeper channel accompanied by a decrease in flow velocity. Examples where these corrections should be considered include flows out of deeper navigation channels onto shallower tidal flats if excess turbulence is generated. Other examples include narrowing flows at the mouth of an estuary, at river passes like those of the Mississippi River, and in flows constricted by a peninsula. Many times submerged sills that cause shallower flows at the entrance of a fjord are associated with points of land that extend into the estuary from both sides. These corrections are obtained from Table 5.25.

4. **Correct for obstructions** - Table 5.24 is used for further correction when large obstructions are contained in the flow (generally expected to cover or occupy approximately one percent or more of the cross sectional area). These include submerged rock outcrops, very large boulders, and small islands (friction losses caused by gradual channel changes around large islands may be unimportant). Rock outcrops and small islands are clearly marked on navigation charts. A very good indication of when corrections are needed is increased turbulence in the flow near the obstruction. From the air, large turbulent eddies are usually very evident when the wind speed is not large.

5. **Correct for vegetation** - If the initial selection does not fully take the effects of vegetation into account, these corrections should be made using Table 5.26. Where vegetation is sparse or patchy, or only extends over part of the depth, it is best to select an initial n value reflective of the sediments in contact with the flow and correct for effects of vegetation using Table 5.26. If vegetation dominates roughness in wetlands and elsewhere, an initial selection from Table 5.22 is best. The initial selection should be compared with corrections in Table 5.26 but should not be modified unless some large discrepancy is noted.

EXAMPLE 5.3. Initial Selection of the Manning n for a Hypothetical Estuary

Table 5.27 illustrates the Manning n selection procedure. Six segments varying from wetland and marsh land, to shallow areas with sea grass, to deep channels with sand, fine grain sediments, and fluid muds were selected for illustration. For segment 1, the initial value was selected as 0.10 from Table 5.22 and corrections were not made for changes in the channel since flow around trees is very irregular and braided and the value from Table 5.22 should account for this. Obstructions (there were very few fallen trees) and vegetation were taken into account in the initial selection. The selection for segment 2 was governed by the same procedure.

Segment 3 involved selection of a value representative of flat sandy bottoms and correcting for the seagrass. The final value should be compared with Table 5.22 where the value is exactly the same as the value for flows over tall grass. Segments 4 and 5 involve straight forward selections for sandy and fine grain materials and minor corrections for changes in cross section and obstructions. Segment 6 involves selection of a smaller value to reflect the influence of fluid mud. The few islands and vegetation on the shores of a wide channel is probably negligible.

Table 5-27. Reach Characteristics for a Hypothetical Estuary and Calculation of the Manning n Value

Segment Number	Description	Bed Material	Bed Topography	Channel Change	Obstructions	Vegetation	n_b	n_1	n_2	n_3	n
1	Wetland with dense stand of straight trees, few fallen trees, very little brush and no weeds	Fine grain	Irregular surface	Meandering. Irregular, braided and indistinct channel in areas	A few fallen trees	See description	0.01	0	0	0	0.01
2	Wetland with marsh grass	na	na	Meandering, Irregular, braided and indistinct channel in areas	None	See description	0.035	0	0	0	0.035
3	Shallow area with sea grass over 70% of the bottom, extending over about 50% of the depth	Sandy	Flat	No significant change	None	See description	0.025	0	0	0.01	0.035
4	Deep well defined channel	Sandy	Dunes	Some narrowing of channel and bends	Submerged	None	0.025	0.01	0	0	0.035
5	Wide deep channel in the vicinity of the turbidity maximum	Fine grain	Ripples	Straight	None	None	0.02	.005	0	0	0.025
6	Wide deep channel down estuary of the turbidity maximum with significant sediment transport into the estuary	Fine grain	Fluid mud layer over much of the channel	Straight	A few small islands	Minor vegetation on the shores	0.015	0	0	0	0.015

EXAMPLE 5.4. Selection of the Manning n for the Delaware Estuary

Figure 1 from Ambrose and Roesch (1982) and Ambrose (1987) shows five zones for the Upper Delaware Estuary. Ambrose and Roesch varied the Manning n in each zone to obtain an optimum fit of predicted water surface elevation to that measured at selected points. The timing of high and low water throughout the estuary was also used to calibrate the model. These data were averaged over a year to filter out the important short-term effect of wind stress that was not included in their hydrodynamics model [Equation (5.10) with the last term for wind stress assumed to be equal to zero on average]. Annual average tidal conditions and fresh inflows were employed. A few measurements of point maximum velocity during ebb and flood tide were compared to the predicted values after calibration but were not used to recalibrate. The result was that n varied from about 0.02 in zone 5 to 0.045 in the riverine dominated zone 1. The value of 0.02 is consistent with a fine grain or sand bed channel with very limited changes in cross section and meandering. The turbidity maximum occurs in this zone. A value of 0.045 in the river zone 1 indicates significant changes in the channel cross section are occurring. Figure 5.8 does not indicate significant meandering. Figure 5.9 shows that excellent agreement was obtained between measured and predicted tidal range for mean tide and average spring tide events. Table 5.7 indicates that discrepancies (as measured by the coefficient of variation) are less than 10 percent throughout the estuary. Thatcher and Harleman (1981) also calibrated a similar model based on Equation (5.17) for the same segments of the Upper Delaware Estuary. They used the same long term average tidal elevation data from the National Ocean Survey (NOS) but also added data from the U.S. Geological Survey (USGS) not used by Ambrose and Roesch (1982) and gave greater emphasis to the USGS data. The n values selected were very similar with one exception in the upper part of the estuary near Trenton where the maximum values of n were selected to be 0.032 versus 0.045 chosen by Ambrose and Roesch (1982). The results from Thatcher and Harleman (1981) are shown in Figure 5.21. The difference could be due to neglecting effects of the longitudinal salinity gradient and by assuming the channel is uniform over five segments. More likely, however, is the emphasis on agreement with two different data sets that are in some conflict. In Figure 5.22, the calibration results of Thatcher and Harleman (1981) for tidal range, and high water and low water planes are shown. The USGS data indicate a larger tidal amplitude in the area of the discrepancy and it is probable that a larger value of n would be necessary to reproduce the larger tidal range measured by the USGS.

Figure 5-21. Longitudinal distribution of Manning n values in the Delaware Estuary (1 mile = 1.61 km) [Thatcher and Harleman (1981)].

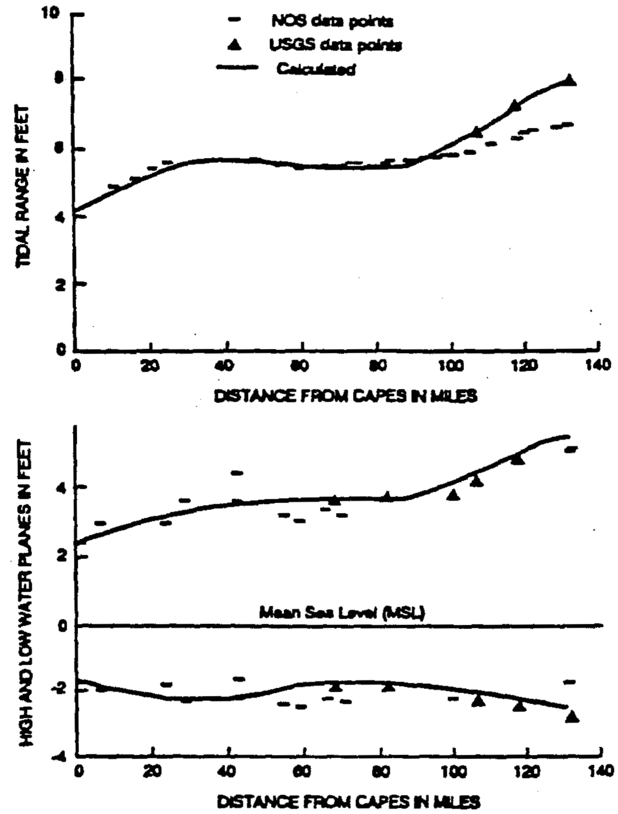


Figure 5-22. Hydraulic calibration to tidal range and high and low water planes for mean conditions (1 ft = 0.035 m; 1 mile = 1.61 km) in the Delaware Estuary [Thatcher and Harleman (1981)].

SUPPLEMENT II: SELECTION OF SURFACE DRAG COEFFICIENTS

The final coefficient necessary to solve Equation (5.17) (hydrodynamics or flow equation) is the water surface drag coefficient that quantifies the effect of wind shear on flow and mixing. As noted above, wind shear is not extremely important for matching predictions with measurements of water surface elevation averaged over long periods of up to a year in deeper tidally controlled estuaries. Ambrose and Roesch (1982), however, note that over periods of hours or days, atmospheric storms can significantly effect water surface elevations on a temporary basis. Shallower estuaries with barrier islands, like the Pamlico-Albermarle Sound, are controlled more by wind shear than tidal influence. As a result, effects of wind shear must be incorporated for shallow tidally damped estuaries when wind driven events cause critical water quality conditions, or when flows are significantly effected by wind during calibration data collection.

For crude estimates, C_{da} is sometimes taken as a constant of about 0.0010 to 0.0025 (Amorocho and DeVries 1980). In general, however, C_{da} is a function of surface roughness and Reynolds number. C_{da} could be determined from Figure 5.23 or a similar friction diagram because of the relationship between various friction factors shown in Table 5.12. But in practice boundary height and air viscosity do not vary significantly and the effect of wind shear on water surface roughness is understood well enough so that a relationship between C_{da} and wind speed can be derived (O'Connor 1983). This relationship is given in Figure 5.23.

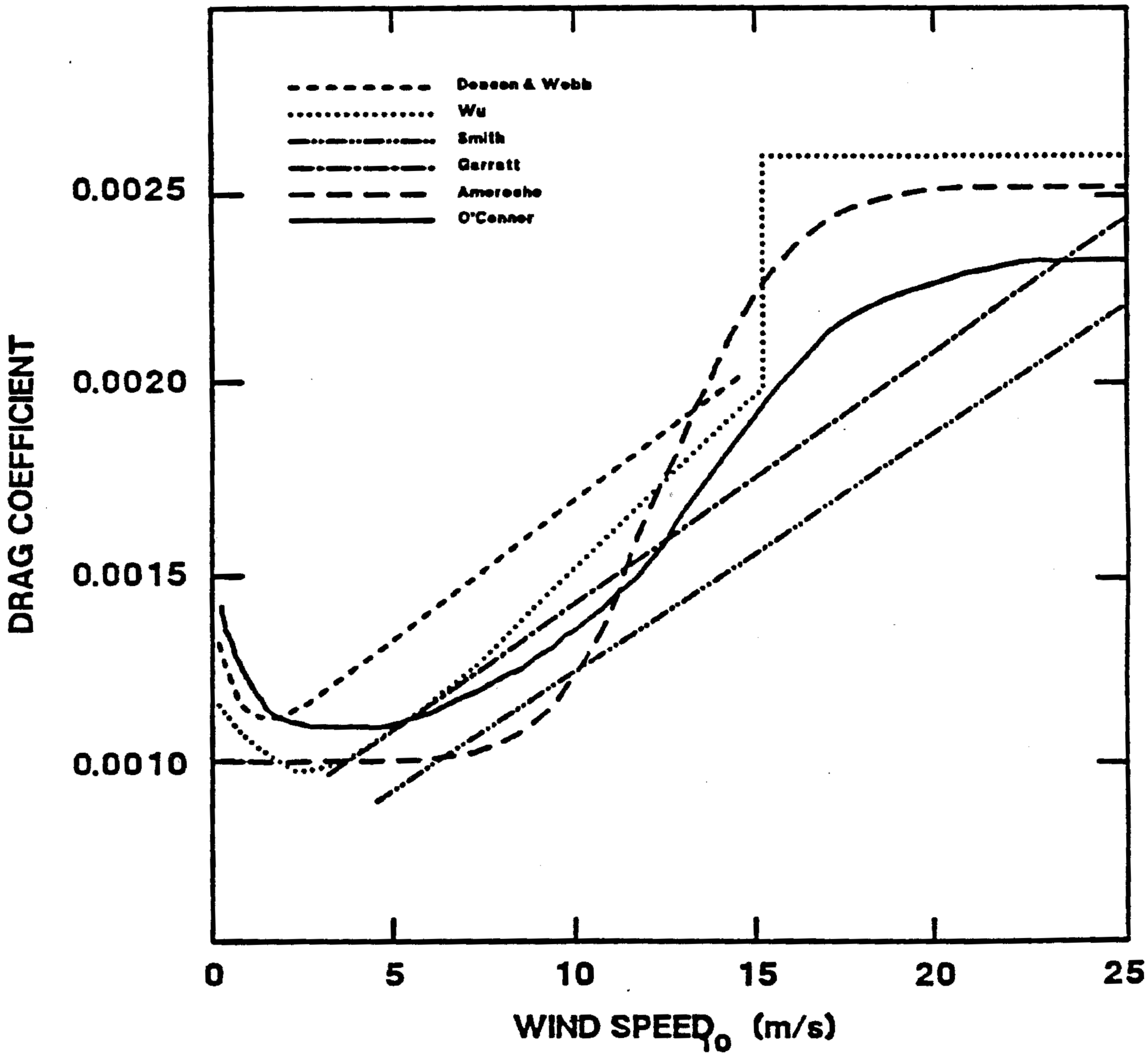


Figure 5-23. Water surface drag coefficient as a function of wind speed measured at a 10-m height [O'Connor (1983)]

SUPPLEMENT III: SELECTION OF EDDY VISCOSITY VALUES

Mixing coefficients required in a typical hydrodynamic model cannot be precisely estimated. Mixing is controlled by flow intensity and estuarine morphology as well as grid resolution and the degree of time averaging employed in the model chosen. These are effects that cannot be forecast sufficiently well to aid in the selection of these parameters. However, initial estimates are needed to begin the calibration procedure. The best guidance available for making the necessary first estimates is found in Bowie et al. (1985) and Fischer et al. (1979). McCutcheon (1983) reviews the commonly used methods of computing vertical mixing.

The initial estimate generally is only required to be close enough to allow the numerical scheme in the hydrodynamic model to converge to a stable solution. Once these estimates are made, fine tuning to achieve precise, optimum estimates of eddy viscosity is rarely necessary. At this time (1989), it is not clear that many simulations of water quality are sensitive to values of the eddy viscosity.

Hydrodynamic models of the eddy viscosity type are limited to describing the effects of large scale turbulent mixing in boundary-layer-like conditions where the turbulence is dissipated under the same conditions in which it was generated. In other words, the effect of localized turbulent mixing in the vicinity of outfalls and associated with diffusers can not be predicted too well in a far-field eddy viscosity model. These effects can be described in calibrating a model, but it is difficult to forecast what eddy viscosity values will be required. At present, a consistent analysis framework that readily links the near-field dilution and mixing analysis (see Chapter 10 in Fischer et al. 1979 and Doneker and Jirka 1988) and the far field eddy viscosity type hydrodynamics models, is not available. To fully understand the basic limitations of the eddy viscosity model and to fully understand when difficulties in selecting calibration values will occur, one should refer to Rodi (1980).

When it seems that water quality simulations are not sensitive to hydrodynamic transport and mixing, the following guidance on the selection of eddy viscosity values should be useful. In some cases, it is expected that hydrodynamic simulations will be important and less approximate methods will be required. In these special cases, higher-order turbulence modeling will be necessary. These special studies will, at present, require expert assistance. To aid in the selection of correct models and expertise, the next Supplement IV will briefly review turbulence closure.

To select eddy viscosity values it should be recognized from inspection of Equations 5.10, 5.11, and 5.12 that eddy viscosity is directly related to the Manning n for certain conditions. As a result, it is assumed that guidance for the selection of eddy viscosity values will be somewhat similar to that developed for the selection of roughness coefficients.

First-order Approximation - As a first approximation, selection of a constant value has proven useful in some studies (see Rodi 1980 for a review). This involves assuming that vertical, lateral, and horizontal eddy viscosities are all equal. From experience with selection of Mannings n in one-dimensional estuaries, values can change significantly along the axis of the estuary. Therefore, this approach should be validated before the results are used in decision making. First, a sensitive analysis of the constant eddy viscosity value on water quality predictions should be performed. Second, validation of the hydrodynamic model should be accomplished by comparing simulations to water surface and velocity measurements. The degree of validation should be matched to the sensitivity of water quality simulations to eddy viscosity values. It should be noted that the model calibrated with a constant eddy viscosity may have only very limited predictive validity outside the range of calibration and validation data.

Typically, a constant eddy viscosity value is only applicable for one-dimensional and two-dimensional depth averaged models where jets and man-made structures do not interfer with the flow (ASCE Task Committee 1988). However, significant phase errors can occur in the prediction of tidal elevations when roughness changes and differences in friction losses are averaged or ignored. Nevertheless, the approximation would seem to be quite useful in wide bodies of water with only limited changes in depth and roughness. Both the lateral and horizontal eddy viscosity is related to a length scale that is approximately equal in many cases.

Constant values have also been applied to models of stratified flows (laterally averaged two-dimensional models and three dimensional models), but these are quite inaccurate. As a matter of practice, constant eddy viscosity values should be avoided except for use in depth-averaged models and crude preliminary or screening level analyses using stratified flow models where the approximation error is well understood and taken into account.

Second-order Approximation for One-dimensional and Depth-averaged Models - To better match tidal elevation measurements, eddy viscosity should be changed in the lateral and horizontal directions to reflect changes in roughness (i.e., bottom roughness element effects), differences in turbulent energy losses (due to "macro-roughness" caused by irregular shoreline bottom morphology), and different scales of the model elements. The Principle of Parsimony should be used, however, to limit changes to those that are absolutely necessary by virtue of well defined and documented changes in roughness, turbulence, and model scale.

When turbulent characteristics of the unstratified estuary do not change extensively, a good depth-averaged model can be reasonably calibrated and expected to make predictively valid simulations over a wider range (compared to the first-order calibration). However, rigorous calibration and validation are normally necessary, especially when water quality results are sensitive to hydrodynamic variables.

Uniform values of the horizontal and lateral mixing coefficients are applied to elements of similar depth and roughness. Values should be increased where turbulence of the flow increases. This includes increases for elements containing separation zones and wakes of flow around islands, headlands, and peninsulas.

Second-order Approximation for Stratified Flow Models - For laterally averaged two dimensional models and three-dimensional models, it is usually possible to obtain a reasonable calibration with a constant lateral and vertical eddy viscosity and by relating the vertical eddy viscosity to a measure of stability such as the Richardson or Froude numbers so that eddy viscosity varies with depth and degree of stratification. This works well for cases where the estuary is relatively deep. Vertical mixing coefficients are typically two or more orders of magnitude smaller than lateral and horizontal coefficients and can be even smaller depending on the degree of vertical stratification (McDowell and O'Connor 1977).

It is especially important that the vertical eddy viscosity formulation be rigiously calibrated (ASCE Task Committee 1988). Generally, stratified flow models using eddy viscosity are not predictively valid outside the range of calibration and validation data. Furthermore, the eddy viscosity and the similar mixing length formulations are only approximately useful for estuarine flows when the flows are approximately boundary-layer like. Complex, unsteady, reversing flows can not be precisely simulated (see Rodi 1980 and ASCE Task Committee 1988).

Third-order Approximation for Three Dimensional Models - The best results for three-dimensional models are obtained when lateral and horizontal values are modified to account for roughness, excessive turbulence production, and model scale, while vertical changes in eddy viscosity are related to depth and stratification. Typically, lateral and hortizontal values are chosen to ensure that changes in tidal elevations are accurately represented and then the vertical eddy viscosity is calibrated to reproduce measurements of vertical velocity and salinity profiles, and longitudinal salinity profiles.

The results should be carefully validated. The predictive validity is not expected to be very good outside the range of calibration and validation data. Generally, eddy viscosity formulations depend upon a critical assumption that turbulence is dissipated under the same circumstances under which it was produced. This is consistently violated in the unsteady salt stratified flows of estuaries and in many cases, more elaborate methods that simulate the generation, transport, and dissipation (under different conditions) of turbulence are required.

Fourth-order Approximation - In a significant number of cases, it is expected that an eddy-viscosity based approach will not be adequate to make predictively valid simulations of critical hydrodynamic conditions nor can eddy viscosity approaches simulate some complex unsteady flows. This is especially true, in some of the larger and very important estuaries in the U.S. These include Cheaspeake Bay and its larger tribuatary estuaries, Long Island Sound and New York Harbor areas, Boston Harbor, Tampa Bay, San Francisco Bay, and Puget Sound to name several. In these cases and others, higher order turbulence closure methods and the necessary expertise are required. Supplement IV briefly reviews the general approach.

Procedurally, the following steps seem to offer the best approach to the calibration of an eddy viscosity type hydrodynamic model (see model equations in Table 2.1 of Part I of this manual -- the values of E_x, E_y, and E_z are to be determined).

A. <u>One-Dimensional Models</u>: See selection of Manning's n, Supplement I

B. <u>Depth Averaged Two Dimensional Models</u>:

1. <u>Estimate a uniform lateral and longitudinal eddy viscosity coefficient for all computation elements</u> (segments or nodes). At least two approaches have proven useful.

a. Empirical length scale formulas (Fischer et al. 1979, Bowie et al., 1985, Bedford 1985) that approximate eddy diffusivity:

$$E_H = 0.005 L^{4/3} \qquad (5.21)$$

where E_H is the horizontal eddy viscosity (lateral, E_y, or longitudinal, E_x) for open waters away from shallow areas and shore and L is the characteristic length scale in centimeters. L is typically taken as the grid size in the model or derived from the physical geometry. For diffusers, L is taken as the diffuser length, which is typically on the order of 1 km. In open estuarine waters, L has been taken as the length of the tidal excursion.

b. Reports of values from similar water bodies. In this regard, the case studies by Officer (1976) provide a useful reference.

2. Correct horizontal eddy viscosity values for areas of higher turbulence. These typically occur in the lee of islands and other shore line irregularities, near the mouth of the estuary, or where bottom roughness changes drastically causing increased velocity gradients.

3. Correct for time averaging. When values from the literature are used, smaller values should be chosen for models with shorter times steps. E_H should be chosen as a larger value in models that average over a tidal period compared to models that average over a much shorter time step.

C. Select vertical eddy viscosity. Table 5.28 from McCutcheon (1983), McCutcheon and French (1985), and others list various formulas that are useful for estimating vertical momentum transfer. Typically a formula is selected and coefficients are modified until calibration is achieved. Predictions of the extent of salinity intrusion into estuaries the existance and location of a halocline and the residence time of pollutants can be quite sensitive to the form and exact magnitude of vertical mixing formulations yet little guidance is available on how these values can be rationally selected. In addition, it is not yet clear what stability parameters (i.e., Richardson number) best quantify the effects of stratification.

1. As Table 5.28 indicates, a number of vertical eddy formulations can be chosen. At present only limited guidance is available to aid in this choice. The formulations listed in Table 5.28 have been used in a number of modeling studies; some (eg., Munk-Anderson) have been used frequently while others have only occasionally been applied. Unfortunately, these model applications have only rarely reported on the usefulness of these formulations. As a result, only crude guidance is possible and that must be derived from a few studies that must also include the data from selected atmospheric boundary layer studies where the stratification effects on mixing are the same in most cases.

2. From the best data available on the Great Ouse Estuary in the United Kingdom (Odd and Rodger 1978), it is clear that the formulations of Holzman and Mamayev are not appropriate for the complete range of stratification encountered in estuaries. These equations are only valid for slight stratification. Knight et al. (1980) shows that the Holzman form is quite inaccurate, especially for large values of Ri (e.g., Ri > 3.4). Also Knight et al. (1980), Nelson (1972) and Delft (1974) tend to indicate that the Mamayev formula is inaccurate, the extreme amount of data scatter not withstanding, and that other forms are better able to be calibrated to represent the data. These conclusions are most important when the RAND two- and three-dimensional hydrodynamic model is being applied. The Mamajev formula was used primarily to provide quick simulated mixing when stratification becomes unstable. As a result, it is not expected that this model will reproduce the vertical structure in estuaries as well as could be expected.

3. Ruling out the Holzman and Mamayev forms leaves the Munk and Anderson [(Rossby and Montgomery 1935) where n = 1 and (Kent and Pritchard 1959) where n = 2)] types of stability functions based on gradient Richardson number as the most adequate. These are most frequently used equations in modeling studies (McCutcheon 1983). However, even these formulations are quite limited and require calibration in all cases. In addition, there is some debate regarding whether other stability parameters are more adequate than the gradient Richardson number. In general, all formulations will not exactly reproduce vertical stratification. Odd and Rodger (1978) and others have found that the Munk and Anderson type formulas only reproduce the general trend of vertical eddy viscosity with changes in stratification as measured by the gradient Richardson number. There are typically large discrepancies in values of β that best fit profiles of E_z measured at different times at a point in the estuary and Table 5.29 shows that there is a significant variation in values determined for different estuaries and other stratified flows. In addition, Odd and Rodger (1978) show that highly stratified

Table 5-28. Vertical Eddy Viscosity Formulations for Flow in Estuaries

Investigator	Formulation for Ez	Comments
Munk and Anderson (1948)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	n = 1 and $\beta(n)$ = 10, based on oceanic thermocline Anderson measurements from Jacobsen (1913) for Rander's Fjord and Schultz's Grund recognized that a general empirical equation could be written.
Rossby and Montgomery (1935)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	n = 1 and $\beta(n)$ = 40, based on Heywood's wind profiles at Leafield. Derived from an energy dissapation per unit volume concept and a flawed assumption that stratified and unstratified velocity gradients are equivalent.
Sverdrup (1936)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	n = 1 and $\beta(n)$ = 10 to 13, based on wind profiles over Spitzbergen snow field.
Holzman (1943))	$E_z = E_{zo}\,[1+\beta(n)\,Ri]$	Empirical equation proposed to explain evaporative flux in the atmosphere. Incorrectly presupposes that a critical Ri of $1/\beta(n)$ exists which is quite inconsistent with the observations of Jacobsen (1913) and others.
Pasquill (1949)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	For n = 1, $\beta(n)$ = 12, and for n = -1 and $\beta(n)$ = -12. From wind profiles in 2-meter layer over grass.
Kent and Pritchard (1957)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	For n = 1, $\beta(n)$ = 2.4; for n = 2, $\beta(n)$ = 0.24; and for n = -1, $\beta(n)$ = 0.06 from tidally averaged data collected in James River Estuary. The semi-empirical formulation for n = 2 was derived from an energy dissapation per unit length (vs. volume) basis with the flawed assumption that stratified and unstratified velocity gradients are equivalent.
Pritchard (1960)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	For n = 2, $\beta(n)$ = 0.28, based on a re-evaluation of the James River Estuary data.
Vreugdenhil (1966)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	For n = 1, $\beta(n)$ = 30, data source unknown.
Nelson (1972)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	For n = 1, $\beta(n)$ = 10; for n = 2, $\beta(n)$ = 2.5 or 5; and for n = -1, $\beta(n)$ = -3.3. Based on data compiled from atmospheric boundary layer including Rider (1954), and Deacon (1955). Also includes inappropriate data from Ellison and Turner (1960).
Odd and Rodger (1978)	1) $E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	For n = 1, $\beta(n)$ = 140 to 180 and for n = 2, $\beta(n)$ = 10 to 15; determined by minimization of relative error from an excellent data base collected in the Great Ouse Estuary. Relative error puts more weight on fit to highly stratified data. Best fit obtained from n = 1 but still the average percentage error in shear stress exceeded 100% for 35% of the measurements.
	2) For Ri continually increasing to over 75% of depth: $E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$ for $Ri \le 1$; $E_z = \frac{E_{zo}}{[1+\beta(n)]^n}$ for $Ri > 1$. For the occurrence of a peak Ri in the lower 75% of the flow at z_o: $E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri(zo)]^n}$ for $Ri(zo) \le 1$; $E_z = \frac{E_{zo}}{[1+\beta(n)]^n}$ for $Ri(zo) > 1$. Except where $E_z > E_{zo}$, then $E_z = E_{zo}$	Better fit to data obtained with a hybrid formula that compensates for the effect of a strong thermocline that accentuates the error in misapplying the eddy viscosity model in estuaries where turbulence is dissipated under conditions different from the conditions generating the turbulence. Best fit is $\beta(1)$ = 160 or $\beta(2)$ = 13. n = 1 remaining somewhat better than n = 2. Improves Reynold stress prediction to $\pm$ 60 for 60% of the data.
Knight et al. (1980)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	Collected additional data in Great Ouse Estuary with less stratification and found that $\beta(1)$ = 110 to 160 and $\beta(2)$ = 13 to 20 consistent with Odd and Rodger (1978).
	$E_z = E_{zo}\,e^{-7.6Ri}$	Formula in poor agreement with Great Ouse Estuary data.
	$E_z = E_{zo}\,[1+\beta(-1)\,Ri]$	Formula in poorest agreement with Great Ouse Estuary data. $\beta(-1) = 3.4$.
Ueda et al. (1981)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$	For n = 2, $\beta(n)$ = 2.5, in the atmospheric boundary layer.
French and McCutcheon (1983)	$E_z = \frac{E_{zo}}{[1+\beta(n)\,Ri]^n}$.	For n = 1, $\beta(n)$ = 30 and for n = 2, $\beta(n)$ = 10 from Great Ouse Estuary analyzed by Odd and Rodger (1978) but the root mean square error was minimized instead of the relative error.

Table 5-28. Vertical Eddy Viscosity Formulations for Flow in Estuaries (continued)

Investigator	Formulation for Ez	Comments
French and McCutcheon (198-) (continued)	$E_z = E_{zo}(1+\alpha k^2 Ro')$	Derived from Monin-Obukhov stability function for atmospheric boundary layer. αk^2 are empirical coefficients determined from unstratified flows (k = 0.41) and from the atmospheric boundary layer (α = 5) such that no calibration is required for estuaries. Limited to small z/L (i.e., $z/L \le 0.0025$); where c = momentum $\overline{\rho' w'} = ck^2z^2(\partial u/\partial z)$ where c = ratio of momentum mixing length to mass mixing length and assumed constant for small z/L; and minimum $\Delta\rho$ is small (i.e., less than 3 to 5%). This form is generally inaccurate like the Holzman (1943) eq. because $Ro' \le (\alpha k^2)$ except for small values of Ro'. Does not fit strongest stratification data from the Great Ouse Estuary at all.
	$E_z = \dfrac{E_{zo}}{(1+\alpha k^2 Ro')}$	Derived from eq. above by noting these eqs. are approximately equal as $\alpha k^2 Ro' \to 0$ and from agreement with data. This equation fits the Great Ouse Estuary data as well as any similar form based on Ri with n = 1 or 2 but αk^2 is known without data fitting from unstratified flows (k = 0.4) and the atmospheric boundary layer (α = 5) and Ro' is less error prone than Ri.
Mamajev (1958)	$E_z = E_{zo}e^{-0.4Ri}$	Based on data of Jacobsen (1913) and reported by author to better fit than other forms. Knight et al. (1980), Nelson (1972), and Delft (1974) show this is inaccurate.
French (1979)	$E_z = \gamma\left[\dfrac{E_{zo}}{1+Ro}\right]^{\Gamma}$	Derived from dimensional analysis and calibrated with Great Ouse Estuary data, γ = 0.062 and Γ = 0.379. This is a grossly empirical eq. that must be calibrated for each estuary of interest and it lacks some vertical resolution because of the definition of Ro.
Henderson-Sellers (1982)	$E_z = \dfrac{E_{zo}}{1+0.74\,Ri}$	Derived from Ueda et al. (1981) atmospheric boundary layer data.
McCutcheon (1983)	$E_z = \dfrac{E_{zo}}{1+\alpha(z/L)}$	α = 5 to 7 (wider range reported is 0.6 to 12 but under questionable experimental conditions.

Notation:

E_{zo} = Vertical eddy viscosity coefficient for unstratified open channel flow = $kzu_*(1 - z/D)$,
k = von Karman's constant assumed to be 0.41,
z = vertical coordinate axis; distance above bottom boundary,
u_* = shear velocity = $(gSD)^{1/2}$ where S is the slope of the energy gradient (or water surface if the flow is approximately uniform),
D = depth of flow (assumed to equal hydraulic radius),
n = exponent for Munk and Anderson stability function; n = 1 for Rossby and Montgomery (1935) function, and n = 2 for Kent and Pritchard (1957) formulation, and n = -1 for the Holzman (1943) formulation.
$\beta(n)$ = constant in the Munk and Anderson stability function for different values of n (i.e., 1,2, and -1) that varies for each estuary and must be calibrated or estimated from other estuaries.

Ri = gradient Richardson number = $-\dfrac{g\dfrac{\partial\rho}{\partial z}}{\bar{\rho}\left[\dfrac{\partial u}{\partial z}\right]^2}$

Ro' = Richardson number based on shear velocity = $-\dfrac{gz^2}{\bar{\rho}u_*^2}\dfrac{\partial\rho}{\partial z}$

Ro_* = gross Richardson number based on shear velocity = $-\dfrac{gD\Delta\rho}{\bar{\rho}u_*^2}$

$\bar{\rho}$ = average density.
g = gravitational constant.
$\partial\rho/\partial z$ = density gradient
$\partial u/\partial z$ = velocity gradient.
α = Monin-Obukhov constant = 5.
$\Delta\rho$ = density difference over the depth of flow.

conditions are difficult to reproduce as others would expect (Munk and Anderson 1948, Henderson-Sellers 1982).

Also, in comparing the results of Kent and Pritchard (1959) based on tidally averaged data, to other studies using profiles that have not been averaged or at least not averaged over periods of more than several minutes (Odd and Rodger 1978, French and McCutcheon 1983, Knight et al. 1980), there seems to be an effect of tidally averaging. If differences between flow conditions in different estuaries are unimportant, the effect of tidal averaging on modeling vertical structure may be up to an order of magnitude of difference in the value of β.

Of the two forms of the Munk-Anderson formula, the Rossby-Montgomery form seems superior to the Kent-Pritchard. This is clearly demonstrated from the studies by Odd and Rodger (1978) and from French and McCutcheon (1983). Perhaps tidally averaged data favors the Kent-Pritchard equation. In addition, French and McCutcheon demonstrate that the Rossby-Montgomery form is less error prone.

The poor predictions from an eddy viscosity formulation are expected in highly stratified flows because the basic concept was developed for uniform flows where turbulence is dissipated under the conditions under which In was generated. When a strong halocline exists in the estuary there is an uncoupling between flow conditions in the lower layers that generate tur-

Table 5-29. Observed Values of the Constants in Various Forms of the Munk-Anderson Stability Function

Source	$\beta(1)$	$\beta(2)$	$\beta(-1)$	Flow condition
Rossby and Montgomery (1935)	40	–	–	Heywood's wind profiles at Leafield
Sverdrup (1936)	10-13	–	–	Wind profiles over Spitzbergen snow field. From Munk and Anderson (1948)
Munk and Anderson (1948)	10	–	–	Oceanic thermocline from Jacobsen (1913) for Randers Fjord and Schultz's Grund
Pasquill (1949)	12	–	12	Wind profiles in 2 meter layer over grass. From Nelson (1972).
Kent and Pritchard (1957)	2.4	0.24	0.06	James River Estuary
Pritchard (1960)	–	0.28	–	James River Estuary
Pasquill (1962)	–	–	2.5 6	Rider's (1954) wind profiles. Taylor's (1960) analysis of Rider's (1954) and eddy flux data of Swinbank (1955)
Vreugdenhil (1966)	30	–	–	Data source unknown. From Nelson (1972)
Nelson (1972)	10	2.5,5.0	3.3	Wind profiles Rider (1955) and questionable pipe flow data from Ellsion and Turner (1960). (1954) and Deacon
Odd and Rodger (1978)	160	13	–	Great Ouse Estuary. Fit by minimizing the relative error.
Knight et al. (1980)	110-160	13-20	3.4	Great Ouse Estuary. Visual fit.
Ueda et al. (1981)	2.5	–	–	Atmospheric boundary layer. From Henderson-Sellers (1982).
Henderson-Sellers (1982)	0.74	–	–	Rederived from data of Ueda et al (1981)
French and McCutcheon (1985)	30	10	–	Great Ouse Estuary. Fit by minimizing the root mean square error.

bulence and the upper layer conditions where some turbulence is dissipated. When the exact stratification structure must be known to determine a waste load allocation or a cause and effect, more elaborate turbulence closure schemes may be required (see Rodi 1980, Sheng (1983), and Blumberg 1977). If vertical structure is repeated during critical conditions, however, it may be possible to calibrate an eddy viscosity model from measurements using the approach of Odd and Rodger (1978) or French (1979) and French and McCutcheon (1983). The choice is governed by whether prediction of highly stratified conditions is more feasible than calibrating an eddy viscosity model with extensive and difficult to collect data.

If calibration is chosen, a number of alternatives are available. First, a site specific equation like that developed by Odd and Rodger (1978) can be developed. Odd and Rodger noted that the Munk-Anderson formula shoud be modified if $Ri \geq 1$ and a significant peak in Ri occurred in the lower 75 percent of the depth of flow. Second, French and McCutcheon (1983) show that less precise, more empirical approaches may yield better results. French (1979) shows that a simpler stability function can be derived by dimensional analysis that uses a gross Richardson number based on shear velocity. French and McCutcheon (1983) found that this simpler equation (see Table 5.28) predicted eddy viscosity better than the complex four equation hybrid model proposed by Odd and Rodgers (1978) that is also given in Table 5.28. Unfortunately, the simplification by French must be calibrated for any use whereas the Odd and Rodger hybrid equation is a direct extension of the Munk-Anderson formulation that may be considered for use without calibration in screening calculations (or at least the Odd-Rodger formulation should be considered before the French equation when calibration is not possible).

The final type of formulation is a class of equations adapted from work in the atmospheric boundary layer using different stability parameters. First, McCutcheon (1983) notes that the most direct application of the atmospheric boundary layer work involves the Monin-Obukhov stability parameter (see Table 5.28). However, the stability parameter z/L where L is the Monin-Obukhov scaling length (Monin and Yaglom 1971), is very difficult to numerically compute even compared to the gradient Richardson number. In addition, there are data (Nelson 1972, Delft 1974) to show that estuaries and coastal areas stratify to a greater degree than the atmospheric boundary layer and strong indications that the layer of constant stress may be less deep in water flows (see Henderson-Sellers 1982). The result is that only limited direct application of the other data for stratified flows is fully feasible. Any application of this sort is limited to small values of Ri.

Second, McCutcheon (French and McCutcheon 1983) shows that the Monin-Obukhov stability function can be converted to a Richardson number (based on shear velocity) function for small z/L. This conversion allows one to maintain the empirical constants determined from extensive measurements (i.e. von Karman constant determined in unstatified flows as 0.4 and α determined as 5 to 7). Unfortunately, the resulting form (see Table 5.28) is of the same inadequate form as the Holzman type equation and has only a limited range of applicability. However, comparison with the Great Ouse data indicates that the proper form should be similar to the Munk-Anderson form, shown as the third equation under French and McCutcheon (1983) in Table 5.28. Further, it can be observed that the constants should retain the same value determined from other conditions (i.e., $k = 0.4$ and $\alpha = 5$). The second two equations under French and McCutcheon (1983) in Table 5.28 must be equivalent in the limit $k^2 \alpha Ro' \rightarrow 0$ according to the procedures generally used to investigate stability functions (Monin and Yaglom 1971). The link between the Monin-Obukhov stability function and the functions derived by McCutcheon are theoretically tenuous but the formulations do as well as any others in describing the vertical mixing in the Great Ouse Estuary and this was accomplished without the extensive calibration required for all other formulations (French and McCutcheon 1983). It is also notable that the parameter Ro' is much less error prone than Ri (e.g., computations of u_* are more precise than those for $\partial u/\partial z$.

As a result, the best methods to represent E_z seem to be the third equation from French and McCutcheon in Table 5.28 or the Rossby-Montgomery equation if the estuary is not strongly stratified. The McCutcheon formulation can be used without calibration in some cases. The value of $\beta(1)$ in the Rossby-Montgomery equation should be taken as about 10 to 30 (see Table 5.29) if calibration is not possible but reduced values of about 2 or 3 may be more useful if tidal averaging is involved or 100 or more if prediction of sharp haloclines ($Ri > 1$) is to be attempted. Calibration to determine α

Table 5-30a. Various Means of Representing the Stability of Stratification and the Relationship between Various Parameters

Parameter	Ri	Ro'	Ro•	Ro	Fr	z/L	R_f	N^2
Definition	$\dfrac{g\frac{\partial\rho}{\partial z}}{\bar{\rho}\left[\frac{\partial u}{\partial z}\right]^2}$	$-\dfrac{gz^2\partial\rho}{\rho u_*^2\partial z}$	$\dfrac{gD\Delta\rho}{\rho U_*^2}$	$\dfrac{gD\Delta\rho}{\rho U^2}$	$\dfrac{U^2}{gD\frac{\Delta\rho}{\rho}}$	$\dfrac{\rho u_*^2}{kg\overline{\rho' w'}}$	$\dfrac{E_z Ri}{D_z}$	$-\dfrac{g\partial\rho}{\rho\partial z}$
Gradient Richardson number, Ri	= Ri	$= \dfrac{Ro'}{k^2\varphi_m^2}$	–	–	–	= z/L for small Ri	$= R_f\varphi_m$	$= \dfrac{N^2}{\left[\frac{\partial u}{\partial z}\right]^2}$
Shear Richardson Number, Ro'	$= Ri(k^2)\varphi_m^2$	= Ro'	= Ro• for $z = D$ and $\frac{\partial\rho}{\partial z} = -\beta$	–	–	–	$= R_f(k^2)\varphi_m^3$	–
Shear Gross Richardson number, Ro•	–	= Ro' for $z = D$ and $\frac{\partial\rho}{\partial z} = -\beta$	= Ro*	–	–	–	–	–
Gross Richardson number, Ro	–	–	–	= Ro	$= Fr^{-2}$	–	–	–
Densimetric Froude number, Fr	–	–	–	$= (Ro)^{-2}$	= Fr	–	–	–
Monin-Obukho Stability pararmeter, z/L	= Ri for small z/L	–	–	–	–	= z/L	–	–
Flux Richardson nymber, R_f .	$= Ri\varphi_m^{-1}$	$= Ro'k^{-2}\varphi_m^3$	–	–	–	–	$= R_f$	–
Brunt-Viasala frequency, N^2	$= Ri\left[\frac{\partial u}{\partial z}\right]^2$	–	–	–	–	–	–	$= N^2$

Notation: β = constant density gradient
ϕ_m = Monin-Obukhov stability function

or β for each individual estuary is presently required if the waste load is sensitive to vertical mixing. Where $Ri>1$, higher order turbulence closure modeling is necessary or extensive calibration of the eddy viscosity model is required if vertical mixing is important.

Finally, these recommendations are specific to the use of the stability parameters Ri and Ro'. A number of hydrodynamic models (McCutcheon 1983) use slightly different forms as given in Table 5.30a. These stability functions should be converted to the required form or the constants corrected as necessary. Table 5.30a gives preliminary guidance on the relationships involved but these have not been thoroughly checked and tested.

SUPPLEMENT IV: BRIEF REVIEW OF TURBULENCE CLOSURE MODELS

In recent years, 2 and 3 dimensional turbulence closure models have been employed in environmental problems (e.g., HYDROQUAL 1987). ASCE Task Committee (1988) gives a good review and assessment of various types of turbulence closure models.

The starting point of all turbulence closure models are Navier-Stokes equations (see Hinze 1975, Rouse 1976, Monin and Yaglom 1971). These equations include all details of turbulence fluctuations, but can only be solved, at present, by introducing time averaged mean quantities. Turbulent quantities are averaged over a time step that is large compared with the time scale of turbulent motion. The equations in Table 2.1 are the result. Averaging and relating the resulting turbulent fluxes to mean flow properties introduces eddy viscosity and eddy diffusivity parameters into the flow and mass transport equations. These coefficients are not related to fluid properties, but are controlled by flow intensity and estuary morphology as well as grid resolution and other factors. The critical steps in turbulence modeling is to relate these turbulent coefficients to average variables (i.e., velocity, pressure, and concentration), empirical constants, and functions, so that this set of equations become a closed set having one more equation than unknown. Turbulence closure models are classified according to how the equations are closed.

Prandtl (1925) suggests that eddy viscosity can be related to the local gradient of mean velocity and a so called mixing length. This theory has been applied and modified by many researchers (e.g., Munk-Anderson 1948, Patanker and Spalding 1970) but mainly in two-dimensional thin-layer flows with only one significant velocity gradient (Rodi 1980). Table 5.28 lists some empirical formulations developed for this theory. As ASCE Task Committee(1988) points out, the mixing length theory assumes that the transport and history of eddy effects can be neglected. It is therefore, not very suitable when these effects are important, as in many estuaries. In some cases, however, mixing length models give reasonably good results when applied to estuaries.

To account for the transport and history of eddy affects, one-equation models have been developed which relate eddy viscosity to turbulent kinetic energy and a length scale (Kolmogorov 1942, Prandtl 1945). The kinetic energy equation (k-equation) was derived from the Navier-Stokes equations which describes eddy energy transport and history. So, theoretically, one-equation models are more suitable than mixing length models when applied in estuaries. But the length scale in this method is not convenient to determine, and can only be determined through empirical equations (Launder and Spalding 1972). Two-equation models have also been develolped and have become more popular based on their greater utility.

Two-equation turbulence closure models introduce one more equation (ε-equation) which is used to determine the length scale. Together with the k-equation (Rodi, 1980), they can account for the transport of turbulent energy and also the length scale of the turbulent motion. They can be used in the situations where the length scale can not be prescribed by empirical equations, and have been applied successfully in many situations where simpler models failed (Rodi, 1980, 1984). But, the length scale equation has been criticized as not universal enough (e.g., Mellor and Yamada, 1982). Also, the k-equation assumes a direct relation between eddy viscosity and eddy diffusivity, and turbulent kinetic energy (which is a velocity scale). In some situations, eddy fluctuations, stress, and the scale used to describe them develop differently. Therefore, more complex stress/flux -equation models have been developed which abandoned the k-equation used by the above two methods. These models are promising in the sense of universality, but are still in the stage of research and have not yet been tested enough (see Rodi 1980, Launder 1984, Mellor and Yamada 1982, Gibson and Launder 1978). So far, turbulence closure models have been employed mainly in the research programs. Though there have been some notable environmental applications (e.g., HYDROQUAL 1987), it should be noted that turbulence models can be reasonably applied only when the model assumptions are not violated, and the extensive requirements for expertise, data, and computation facilities are met. Presently, cost compared with the benefits might make it unfeasible to employ a turbulence closure model in a particular estuary waste load allocation study. Hopefully, this will change the near future. For more detailed turbulence model descriptions, one can consult ASCE Task Committee (1988), and Rodi (1980).

It is a good suggestion that one use one-dimensional hydrodynamic models, which lump turbulence effects into a simple roughness coefficient discussed in Supplement I and are throughly tested, much easier to implement and well documented, whenever possible. If it is decided that a turbulence model should be used, one should be fully aware of the expertise and cost required.

SUPPLEMENT V. SELECTION OF DISPERSION COEFFICIENTS

Dispersion coefficients are empirical analogs of the molecular diffusion coefficient defined in the advective-diffusive equation:

$$\frac{\partial C}{\partial t} + \frac{\partial (UC)}{\partial x} + \frac{\partial (VC)}{\partial y} + \frac{\partial (WC)}{\partial z}$$

$$= D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} + \Sigma S \tag{5.22}$$

where C is concentration of the constituent being modeled; U, V, and W are mean water velocities in the x, y, and z coordinate directions, respectively; and D_x, D_y, and D_z are the longitudinal, lateral and vertical dispersion coefficients, respectively. ΣS is the sum of all sources and sinks of constituent C. Typical values of longitudinal, lateral, and vertical turbulent dispersion are much larger than values of thermal and molecular diffusion as shown in Figure 5-24.

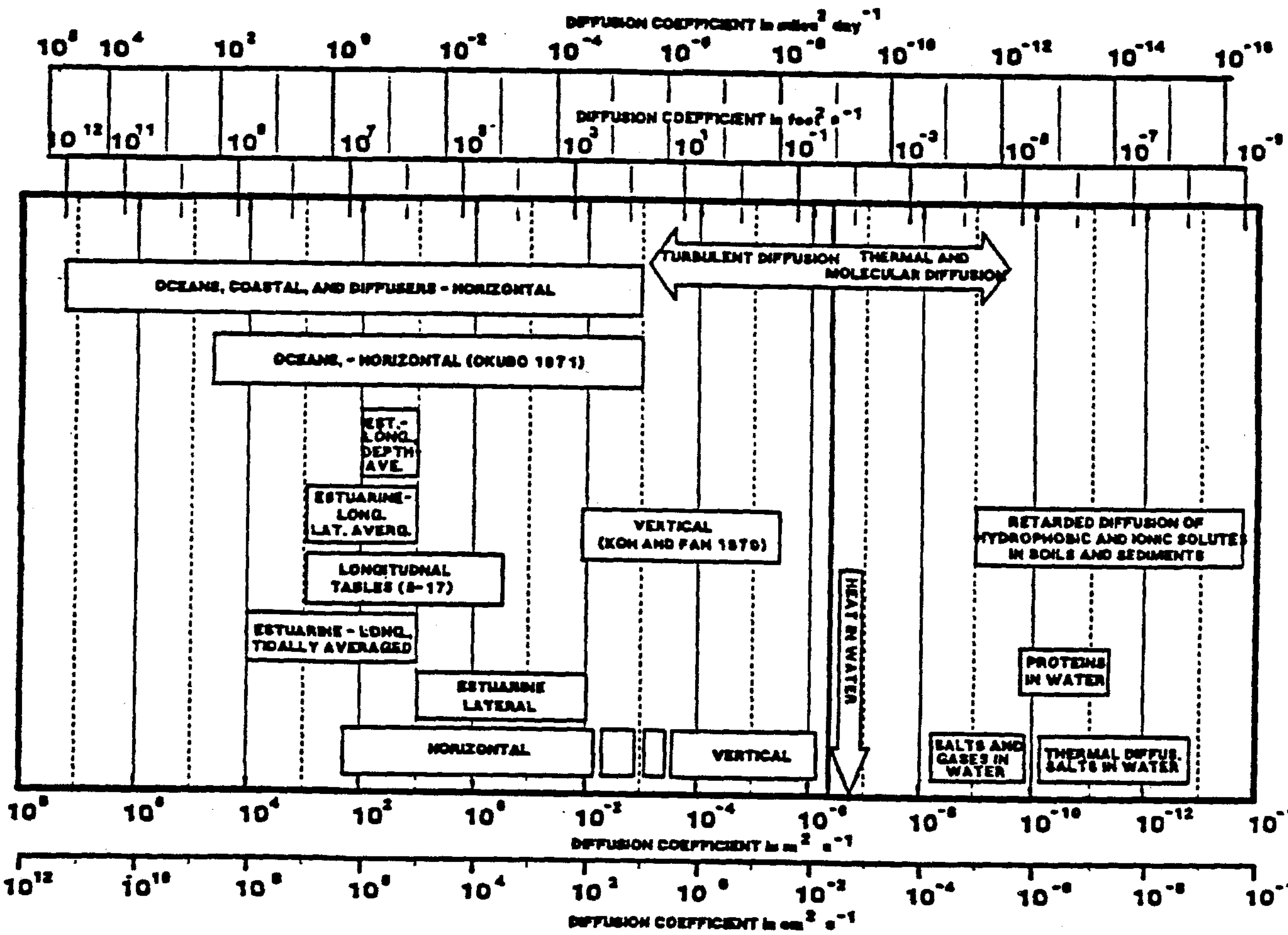


Figure 5-24. Diffusion Coefficients.

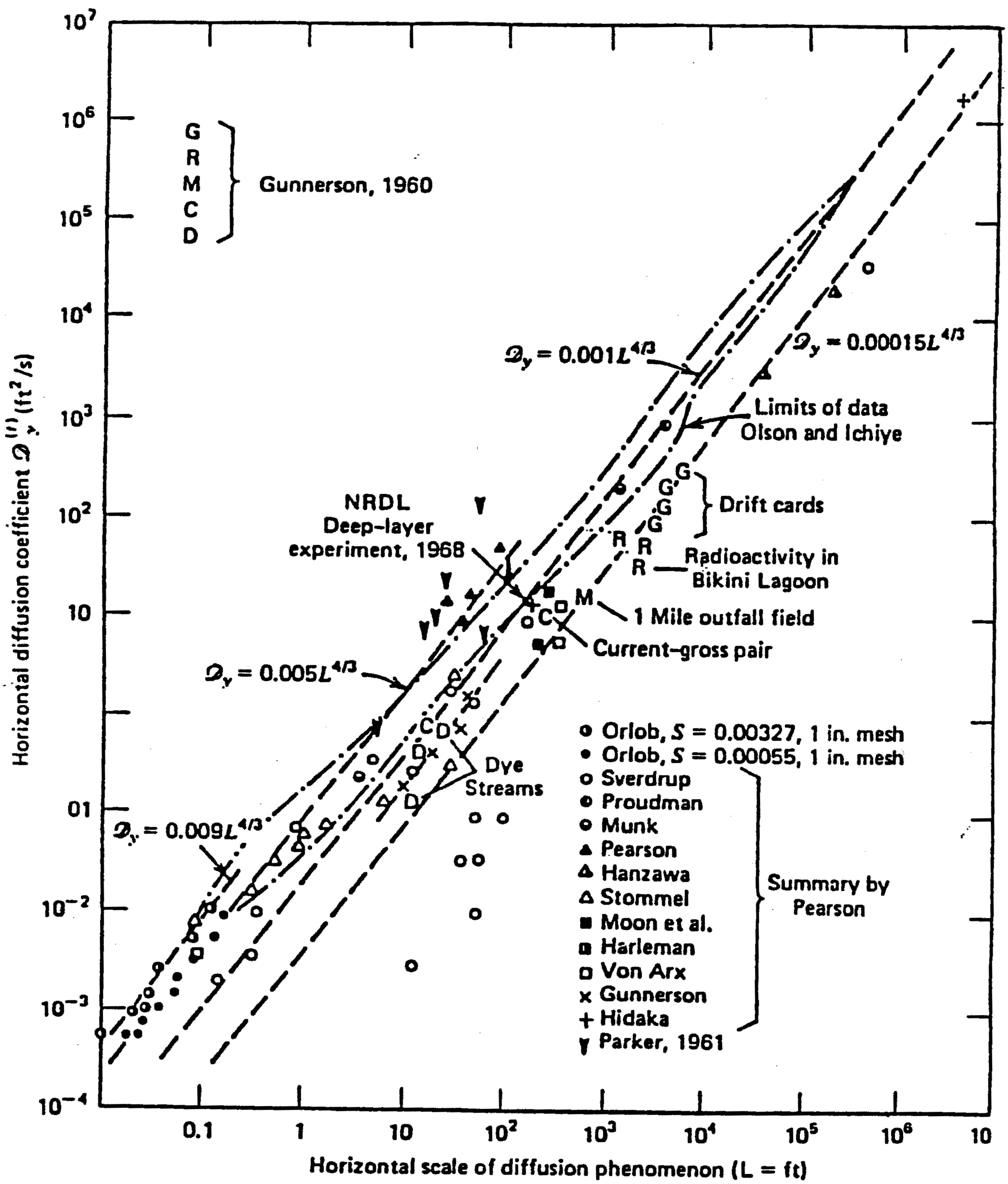


Figure 5-25. Relationship between horizontal diffusion coefficient and horizontal length scale [Thibodeaux (1979), Fan and Koh, Orlob (1959), Okuba].

The dispersion coefficients can not be defined in terms of physical properties of the water. These represent coefficients of proportionality relating velocity gradients ($\partial U/\partial x$, $\partial V/\partial y$, and $\partial W/\partial z$) to correlations of turbulent fluctuations of concentration, c', and velocity (u', v', and z') written as: $\overline{u'c'}$, $\overline{v'c'}$, and $\overline{w'c'}$ (McCutcheon 1989). As such, the coefficients of proportionality represent a method of simplifying the transport equation so that it may be reasonably solved. The dispersion coefficients are therefore, functions of turbulence ($\overline{u'c'}$, $\overline{v'c'}$, $\overline{w'c'}$), which in turn are related to flow conditions in the estuary, and the method of averaging over time or space. Greater numerical dispersion and thus lower actual specified dispersion results when the equations are solved over greater element distances or averaged over longer time periods. The coefficients can not be predicted but a number of empirical relationships have been observed that can be used to estimate initial values. In addition, there are a number of case studies that establish representative values. These initial values are then modified as necessary to calibrate the model.

When estimating the dispersion coefficients, it should be noted that these are empirical factors that are not only related to the turbulence in the flow but that these values are also influenced by the way in which Equation 5.22 is solved. Therefore, at least minor differences are expected to be found if different numerical schemes, with differing degrees of numerical dispersion are employed, or if different length and time scales are used in solving the equations. As a result, any observational experience obtained from similar estuaries or from predictive equations based on past experience, are useful as initial guidance but may not be adequately related to the conditions in the estuary being simulated with the form of Equation 5.22 in the model being used. This includes use of eddy viscosity values obtained from prior calibrations of different models in the estuary of interest where some difference may occur between the final calibrated values and the previous estimates. In addition, the use of case studies from other estuaries must be carefully considered to be sure that the calibrated model was sensitive to the dispersion coefficients. If the calibrated model was not sensitive to the dispersion coefficients, the final values may not be estimated precisely.

Generally, concentration distributions in estuaries and streams are not sensitive to dispersion coefficients (Krenkel and Novotny 1980). Therefore, precise calibration usually is not critical.

The general guidance is somewhat similar to that used for the selection of eddy viscosity values and is as follows:

1. Qualitatively estimate relative importance of mixing by various mechanisms. These mechanisms include shear flows set up by tides and river flow, mixing by wind shear, and mixing by internal density differences. The importance of these mechanisms indicates how best to select dispersion coefficients. Various methods include:

   a. Estimation of shear flow dispersion. Fischer et al. (1979) notes that dispersion can be reasonably estimated in estuaries that are long and narrow, or wide. Shear flow dispersion, usually acting along the longitudinal axis of the estuary, is most important when mixing times across the estuary are approximately equivalent to times required to mix along the axis of the estuary (Fischer et al. 1979). Fischer et al. (1979) note that the maximum longitudinal dispersion due to shear is approximately

   $$K_x = 0.1(0.2\,U^2)T\,(0.8) \qquad (5.23)$$

   Where K_x is expressed in $m^2\,s^{-1}$, (0.2U) is assumed to approximate the deviation of the velocity in a cross section from the cross sectional average, T is the tidal period in seconds, and the constant 0.8 is derived by Fischer et al. (1979, see their Figure 7.4). U is the mean tidal velocity. Fischer et al. (1979), illustrates this method of estimation.

   b. Fraction of freshwater method. Officer (1976) describes how freshwater and observed longitudinal salinity gradients can be used to estimate longitudinal dispersion.

   c. 4/3's law. It has been widely observed that lateral dispersion can be estimated from the empirical formula:

   $$K_y = constant\ (length\ scale)^{4/3} \qquad (5.24)$$

   See Bowie et al. (1985), Officer (1976), and Figure 5.25.

2. Compare estimates with published values. Tables 5.30b, 5.31, and 5.32 compile the readily available estimates of tidally averaged longitudinal coefficients, longitudinal dispersion coefficients observed in two-dimensional estuaries and coastal waters, and lateral dispersion coefficients. These values should be used to confirm the reasonableness of estimates made with Equations 5.23 and 5.24 or to provide preliminary estimates for the water body of interest. See Officer (1976).

Table 5-30b. Tidally Averaged Longitudinal Dispersion Coefficients Observed in Selected One Dimensional Estuaries [Hydroscience (1971), Officer (1976) and Bowie et al. (1985)]

Estuary	Freshwater Inflow (m^3s^{-1})	Freshwater Inflow (ft^3s^{-1})	Low Flow Net Non-tidal Velocity (ms^{-1})	Low Flow Net Non-tidal Velocity (fts^{-1})	Longitudinal Dispersion Coefficient (m^2s^{-1})	Longitudinal Dispersion Coefficient (ft^2s^{-1})	Comments
North America							
Hudson River Mouth	106 to 637	3,750 to 22,500	-	—	450 to 1,500	4,840 to 16,133	From O'Conner (1962). Found correlation between flow and Kx
Potomac	56	2000	—	—	6 to 59	65 to 635	Estimated from the fraction freshwater method and dye studies by Hetling and O'Connell (1965, 1966). A very consistent relationship between Kx and distance downstream of Chain Bridge observed
San Francisco Bay							
Suison Bay	—	—	—	—	600 to 1,400	600 to 15,000	Determined by Bailey (1966) from dye studies of one to a few days in duration.
Sacramento and San Joaquin Rivers	—	—	—	—	9 to 90	100 to 1,000	
Northern Arm	—	—	—	—	30 to 1,770	320 to 19,000	Determined with the fraction of freshwater method by Glenne and Selleck (1969) from measurements over 3 stages of the tidal cycle at 2 or more depths. Glenne and Bailey also used silica as a conservative tracer and confirmed that values of Kx were accurate.
Southern Arm	—	—	—	—	10 to 100	190 to 1,900	
Yaquina	17	—	—	—	60 to 853	650 to 9,180	Burt and Marriage (1957) determined these values by fraction of freshwater method. High flow Kx significantly higher than low flow Kx.
	low flow	—	—	—	14 to 99	140 to 1,066	
United Kingdom							
Narrows of Mersey	25.7	907.6	—	—	161	1,733	Estimates based on the fraction freshwater method measured at various locations along with salinity concentrations averaged over tidal cycles.
	103	3,637	—	—	359	3,864	
Severn	—	—	—	—	54 to 174	581 to 1,873	Kx values recomputed by Bowden (1963) from estimates of Stommel (1953). Bowden included the freshwater inflow from tributaries in the fraction of freshwater method and derived significantly larger values. The higher values are representative of a section with a tidal bore.
Southampton					158	1700	Kx computed by fraction freshwater method by Dyer (1973).
Thames	low flow	—	—	—	53	570	At 16 Km (10 miles) and 40 Km (25 miles) downestuary of London Bridge.
					84	904	
	high flow	—	—		338	3,638	At 48 Km (30 miles) downestuary of London Bridge.
Tay	50	1,766	—	—	50 to 135	540 to 1,453	Estimates by the fraction freshwater method. Estimated by the fraction freshwater method. Kx varies at each location as a function of freshwater discharge.
	100	3,531			70 to 210	750 to 2,260	
	200	7,063			30 to 470	320 to 5,060	
	300	10,600			70 to 700	750 to 7,530	
Japan							
Ariake Bay	—	—	—	—	670	7,212	Derived by Higuchi (1967) from an observed longitudal salinity profile caused by freshwater inflow of the Chikugo River. Diffusion of small dye patches were found to follow the 4/3's law.

Table 5-31. Longitudinal Dispersion Coefficients Observed in Selected Two Dimensional Estuarine and Coastal Water Studies [Hydroscience (1971), Officer (1976) and Bowie et al. (1985)]

Estuary	Freshwater Inflow (m^3s^{-1})	Freshwater Inflow (ft^3s^{-1})	Low Flow Net Non-tidal Velocity (ms^{-1})	Low Flow Net Non-tidal Velocity (fts^{-1})	Longitudinal Dispersion Coefficient (m^2s^{-1})	Longitudinal Dispersion Coefficient (ft^2s^{-1})	Comments
United Kingdom							
Irish Sea	—	—	0.0035	0.0115	500 to 900	5,380 to 9,690	Estimated from the longitudinal salinity gradiental across a section between Lands End and Cape Clear and between St. Davids Head and Carnsore Point using the simplified continuity relationships known as Knudsen's relations. Large values attributable to large depths and extremely large horizontal length scales.
North Sea	—	—	—	—	21.7 to 9.6	234 to 103	Estimated from dye spreading experiments with instantaneous point injections tracked for up to 60 hr. $K_x = \sigma_x/2t$.
Firth of Fal	—	—	—	—	0.4 to 3.6	4.3 to 38.9	Estimated from dye spreading experiments with instantaneous point injections tracked for up to 7 hr. $K_x = \sigma_x/2t$.
Blackwater	—	—	—	—	13 to 27	140 to 291	Estimated from dye spreading experiments with instantaneous point injections tracked for up to 12 hrs. $K_x = \sigma_x/2t$.
Japan							
Osaka Bay and Mizushima Bay	—	—	—	—	0.5	5.4	Determined by calibration of a heat balance model for thermal plume injected into the bay from a power plant.
Ariake Bay	—	—	—	—	0.25 to 5	2.7 to 53.8	Determined by Higuchi (1967) from diffusion of small dye patches in the bay. The data follows the 4/3's law.

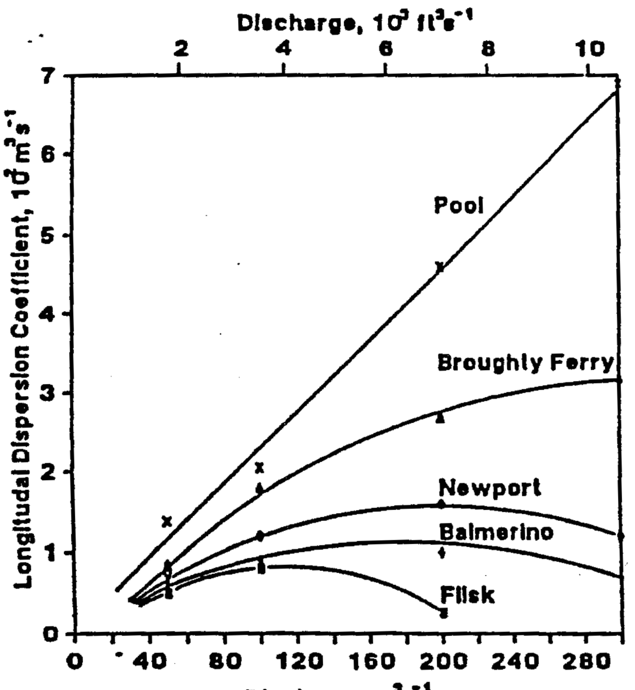


Figure 5-26. Relationship between longitudinal dispersion coefficient and discharge in a Scottish estuary [West and Williams (1972)].

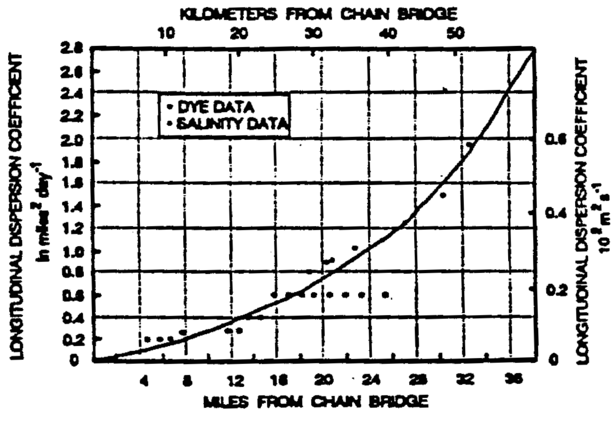


Figure 5-27. Relationship between longitudinal dispersion coefficient in the Potomac Estuary and distance downestuary from the Chain Bridge in Washington, D.C. [Hetling and O'Connell (1966)].

Table 5-32. Lateral Dispersion Coefficients in Estuaries and Coastal Waters [Officer (1976)]

Estuary	Lateral Dispersion Coefficient (m^3s^{-1})	(ft^3s^{-1})	Comments
			United Kingdom
Severn Estuary	2	22	Estimated by de Turville and Jarman (1965) from the mixing of the thermal plume entering the estuary with the River Usk into the Bristol Channel using observed temperature distributions, cooling water flow rates, river flow rates, and assumptions about the distribution of the sources at the outfall. Ky was related to the lateral dimensions of the river.
Fal Estuary	1.5	16	Estimated from dye spreading perpendicular to the axis of longitudinal spreading of an instanteous point injection. Spreading occurred over periods of up to 7 hrs. Ky = $\sigma y/2t$.
Blackwater Estuary	3 to 9	32 to 97	Estimated from dye spreading perpendicular to the axis of longitudinal spreading of an instantaneous point injection. Spreading occurred over periods of up to 12 hrs. Ky = $\sigma y/2t$.
North Sea (between U.K. and Europe)	1.4 to 6.0	15 to 65	Estimated from dye spreading perpendicular to the axis of longitudinal spreading of an instanteous point injection. Spreading occurred over periods of up to 12 hrs. Ky = $\sigma y/2t$.
Irish Sea (between U.K. and Ireland)	110 to 1,480	1,184 to 15,930	Based on a simple heat balance by Bowden (1948).
	25	270	Based on a steady-state salt balance and assumptions that the longitudinal salinity gradient through the Sea is linear, the lateral gradient is parabolic, the vertical salt balance terms are negligible, lateral advection can be neglected, and the horizontal advective velocities are on the order of 0.005 m s^{-1} (0.016 ft s^{-1}).
			Japan
Osaka Bay and Mizushima Bay	0.5	5.4	Determined by calibration of a heat balance model for a thermal plume injected into the bay from a power plant.

3. Correct for areas of higher turbulence. These areas typically occur in the lee of islands and other shore line irregularities or where bottom roughness or topography changes drastically.

4. Relate dispersion coefficient to freshwater discharge. If the waste load allocation covers more than a single freshwater discharge condition, longitudinal dispersion coefficients are typically related to changing freshwater discharge as illustrated in Figure 5.26.

5. Relate dispersion coefficient to location. The longitudinal dispersion coefficient tends to increase in the downestuary direction. See Figure 5.27 for an illustration of the expected behavior.

6. Select vertical dispersion coefficients. McCutcheon (1983) lists various formulas that are useful. Typically a formula is selected and modified if necessary during calibration. See guidance on the selection of vertical eddy viscosity.

Table 5-33. Evaporation Formula for Lakes and Reservoirs [Ryan and Harleman (1973)]

Investigator	Evaporation Rate Expression In Original Form	Units* for E, u, and E*	Observation Levels	Time Scale Increments	Water Body	Formula at Sea Level**	Remarks
Marcians and Harbeck (1954)	$E = 6.25 \times 10^{-4} u_8 (e_o - e_8)$	$cm (3\ hr)^{-1}$ knots mb	8m-wind 8m-e_a	3 hrs Day	Lake Hefner, Oklahoma 2587 acres	$12.4 u_8 (e_o - e_8)$ $17.2 u_2 (e_o - e_2)$	Good agreement with Lake Mead, Lake Eucumbene and Russian Lake data.
Kohler (1954)	$E = 0.00304 u_4 (e_o - e_2)$	$in. (day)^{-1}$ $miles (day)^{-1}$ in. Hg	4m-wind 2m-e_a	Day	Lake Hefner, Oklahoma 2587 acres	$15.9 u_4 (e_o - e_2)$ $17.5 u_2 (e_o - e_2)$	Essentially the same as the Lake Hefner Formula.
Zaykov (1949)	$E = [.15 + .108 u_2](e_o - e_2)$	$mm (day)^{-1}$ ms^{-1}, mb	2m-wind 2m-e_a		Ponds and small reservoirs	$(43 + 14 u_2)(e_o - e_2)$	Based on Russian experience. Recommended by Shulyakovskiy.
Meyer (1942)	$E = 10(1 + 0.1 u_8)(e_o - e_8)$	$in. (month)^{-1}$ 25 ft-wind mph in. Hg	25 ft - wind 25 ft-e_a	Monthly	Small lakes and reservoirs	$(73 + 7.3 u_3)(e_o - e_8)$ $(80 + 10 u_2)(e_o - e_2)$	e_a is obtained daily from mean morning and evening measurements of T_a, and relative humidity. Increase constants by 10% if average of maximum and minimum used
Morton (1976)	$E = (300 + 50 u_8)(e_o - e_a)/p$	$in. (month)^{-1}$ mph in. Hg	8m-wind 2m-e_a	Monthly	Class A pan	$(73.5 + 12.2 u_8)(e_o - e_2)$ $(73.5 + 14.7 u_2)(e_o - e_2)$	Data from meteorological stations. Measurement heights assumed.
Rohwer (1931)	$E = 0.771[1.465 - .0186B] \times [0.44 + 0.118u](e_o - e_a)$ where B = atmos. press	$in. (day)^{-1}$ mph in. Hg	0.5-1 ft-wind 1 inch-e_a	Daily	Pans 85 ft diameter tank 1300 acre reservoir	$(67 + 10 u_2)(eo - e_2)$	Extensive pan measurements using several types of pans Correlated with tank and reservoir data.

* For each formula, the units are for evaporation rate, wind speed, and vapor pressure (i.e., in Meyer's formula evaporation rate is in inches month $^{-1}$, wind speed is in miles per hour (mph) measured 25 feet above the water surface, and vapor pressure is in inches of mercury also measured at 25 feet).

** Measurement heights are specified as subscripts to wind speed, u, and vapor pressure, e. The units for evaporation rate, E; wind speed; and vapor pressure or saturation vapor pressure (e_a and e_o) are BTU $ft^{-2} day^{-1}$, miles hr^{-1}, and mm Hg, respectively

SUPPLEMENT VI: SELECTION OF WIND SPEED FUNCTIONS:

All mechanistic temperature models have at least one empirical function, known as the wind speed function, that must be specified during the calibration procedure. Even equilibrium temperature approximations have the wind speed function embedded in the first-order heat transfer coefficient (McCutcheon 1989). The wind speed function is typically expressed in Stelling's form (Brutsaert 1982) as:

$$E = (a + b u_w)(e_o - e_a) \qquad (5.25)$$

where E is the heat flux due to evaporation, $(a + bu_w)$ is the wind speed function to be specified as part of the calibration procedure, and $e_o - e_a$ is the difference between the saturation vapor pressure of the atmosphere at the ambient temperature (e_o) and the measured vapor pressure (e_a).

Whether the waste load allocation is sensitive to the choice of wind speed coefficients or not determines how precise the calibration must be. Generally, the final results are not expected to be overly sensitive to temperature predictions. Temperature gradients are normally not as strong as salinity gradients and changes in temperature over the estuary do not seem likely to cause large differences in biochemical reactions. The wind speed function, therefore, is expected to be most important when simulations extend over seasonal changes (i.e., spring into summer) and when the evaporative heat flux is a significant part of the estuary heat balance.

Typically, a wind speed function is selected from the compilations of available functions given in Tables 5.33 and 5.34. The best choice from the compiled values is one that has been developed for a water body of similar size at approximately the same latitude. Shore line conditions that influence aerodynamic roughness and the atmospheric boundary layer over the estuary should be similar if possible. When the wind speed function is modified during calibration, it is usually best to change the function by a constant multiplier rather than arbitrarily changing the coefficients a and b (McCutcheon 1989) by disproportionate amounts unless the physical meaning of the two coefficients is well understood (e.g., see Wunderlich 1972, Ryan and Harleman 1973).

Table 5-34. Evaporation Formulas [Wunderlich (1972) and McCutcheon (1989)]

Investigator	Evaporation Rate Expression $E=f(u, e_o, e, etc.)$	Units for E, u, & e	Time Scale	Type of Water Body
Penman (1956)	$0.35(0.5+0.01u_2)(e_o-e_2)$	mm day^{-1} mi/day @ 2m mm Hg	-	Lake, meteorological data collected on land
Meyer (1942)	$0.36(1+0.1u_{7.6})(e_o-e_{7.6})$	in. month^{-1} mph @ 7.6m in. Hg	Daily	Small lakes, reservoirs, and pan evaporation
Harbeck et al. (1958)	$0.078u_2(e_o-e_2)$	in. day^{-1} mph @ 2m in. Hg	Daily	Lake Mead, NV
Turner (1966)	$0.00030u_2(e_o-e_2)$	ft. day^{-1} mph @ 2m in.Hg	-	Lake Michie, NC
Fry	$0.0001291u_2(e_o-e_2)$	cm. day^{-1} km. day^{-1} @ 2m mb	-	-
Easterbrook (1969)	$0.000302\ u_2(C_o-C_2)$ $0.000001942\ u_2(C_o-C_2)$ C is relative humidity, unitless	g cm^{-2} s^{-1} ft. s^{-1}	-	Lake Hefner, mid-lake Lake Hefner combined data
Jobson (1980)	$(3.01 + 1.13u_2)(e_o-e_2)$	mm day^{-1} ms^{-1} @ 2m kilopascals	-	San Diego Aqueduct, CA. Energy balance.
Faye et al. (1979)	$0.70(3.01 + 1.13u_2)(e_o-e_2)$	mm day^{-1} ms^{-1} @ 2m kilopascals	-	Chattahoochee River, GA.
McCutcheon (1982)	$0.45(3.01 + 1.13u_2)(e_o-e_2)$	mm day^{-1} ms^{-1} @ 2m kilopascals	15 min	West Fork Trinity River, TX.
Fulford and Strumm (1984)	$(0.032 + 0.008u_2)(e_o-e_2)$ or $(0.012\Delta\theta^{1/3} + 0.013u_2)(e_o-e_2)$ $(0.024 + 0.006u_2)(e_o-e_2)$ or $(0.010\Delta\theta^{1/3} + 0.007u_2)(e_o-e_2)$ $\Delta\theta$ is the virtual temperature difference between air and the water surface.	cm day^{-1} ms^{-1} @ 2m kilopascals	2 hrs	Small Channel at ambient temperatures. Decatur, AL. Small Channel at elevated temperatures. Decatur, AL.

SUPPLEMENT VII: SELECTION OF BACTERIA DIE-OFF COEFFICIENTS

Traditionally, the bacteria die-off process is considered as a simple first-order decay, such that

$$\frac{dN}{dt} = -K_B N \qquad (5.26)$$

where N = bacteria concentration {num/L^3}
Kв = die-off or decay rate {1/T}

The resulting distribution downstream is

$$N = N_0 e^{-K_B t}$$

where

N_o = initial concentration of bacteria {num/L^3}

In some cases, bacteria resuspension from the bottom can be important, so, a resuspension term is added

$$\frac{dN}{dt} = -K_B N + \frac{V_u}{H} M_s R_N \qquad (5.27)$$

where

V_u = resuspension velocity {L/T}
H = water column depth {L}
M_s = solids concentration in the sediment {M_s/L^3}
R_N = bacteria concentrations based on solids {num/M_s}

The solution of equation 5.21 is

$$N = N_o ext(-K_B t) + \frac{V_u M_s R_N}{H K_B}[1 - e^{-K_B t}] \qquad (5.28)$$

For bacteria analysis and modeling, the order of magnitude is often considered precise enough, so, steady state modeling is often employed. On the other hand, the fate of bacteria in natural waters is assumed to be a first-order decay, therefore all modeling procedures for other contaminants with a first-order decay are applicable to bacteria.

Table 5.35 and 5.36 compile the bacteria decay rates from studies involving salty and fresh waters, respectively. They can be used as a guidence to select initial rates for a particular study. Generally, the decay rates for coliforms are on the order of 1 per day, but can be as high as 48/day for marine outfalls. Virus decay rates are usually one order of magnitude lower than that of bacteria.

In estuaries and other natural water bodies, the fate of bacteria is affected by many site-specific factors, such as (Thomann and Mueller 1987, Bowie, et.al., 1985) temperature, sunlight, salinity, settling, resuspension, aftergrowth, nutrient difficiencies, predation, and toxic substances. After selecting a initial value for the decay rate, adjustment should be made to fit the prediction results to actual measurement by trial and error. Often, the actual bacteria decay is not exactly first-order. Under these situations, the decaying process is divided into different stages. Each stage can be described reasonably well by first-order decay and a different decay rate (Thomann and Mueller 1987).

An alternative way of selecting the initial bacteria decay rate is described in Thomann and Mueller (1987). They recommend an empirical equation which includes the effects of salinity, temperature, sunlight and settling of bacteria.

$$K_B = [0.8 + 0.006(\%seawater)]\, 1.07^{T-20} + \frac{\alpha I_0(t)}{K_e H}[1 - e^{-K_e H}] + \frac{V_s}{H} \qquad (5.29)$$

where

% sea water = percent of salinity compared to sea water
1.07 = temperature correction coefficient
T = temperature in °C
α = constant coefficient in light correction function
I_o = surface solar radiation, Cal/m^{2}hr
K_e = vertical light extinction coefficient in water column, 1/m
V_s = settling velocity of particulate bacteria in m/day. Precisely, V_s should not include resuspension, which is already accounted for with a resuspension term in Eq. 5-22. But, lumping resuspension into V_s is also feasible; then V_s becomes net settling rate.

H = water column depth, m.

Following is a simple example to calculate bacteria transport.

T = 25°C
Q = 200 m^3/sec
u = 0.01 m/sec
E = 50 m^2/sec
Discharge: 0.5 m^3/sec, 4 x 10^6 FC/100ml
x = 5 km to bathing area
S_o = 7 PPT

Where PPT = part per thousand and FC is the number of fecal coliform bacteria. The problem is the water quality standard requires the fecal coliform bacteria concentrations in a bathing area to be less than 200/100 ml. If an effective aftergrowth factor is as-

Table 5-35. Reported Decay Rate Coefficients for Bacteria and Viruses in Seawater and Brackish Water [Thomann and Mueller (1987), Bowie et al. (1985), and Velz (1984)]

Organism	Dieoff Rate Coefficient * (d^{-1} base e)	Temperature (°C)	Reference	Comments
Coliforms:				
Total coliform	1.4 (0.7 to 3.0)	20	Mancini (1978)	Seawater
	48. (8. to 84)	—	Mitchell and Chamberlain (1978)	Collected from 14 ocean outfalls, variable temp.
Total or fecal coliform	0.0 to 2.4	—	Hydroscience (1977b)	New York Harbor Salinity: 2 to 18 o/oo. Sample kept in darkness
	2.5 to 6.1	—	Hydroscience (1976b)	New York Harbor Salinity: 15 o/oo. Sample kept in sunlight
	0.48	20	Chen (1970)	Derived from the calibration of a model for San Francisco Bay
	0.48 to 8.00	20	Tetra Tech (1976)	Derived from model calibration for Long Island, New York Estuaries
	1.0 (summer)	—	Velz (1984)	Observed in New York Harbor
	0.60 (summer)	—	Velz (1984)	Moracaibo Strait, Venezula; from observations by Parra Pardi.
Fecal coliform	37 to 110		Fujioka et al. (1981)	Seawater kept in sunlight
E. coli	0.08 to 2.0	—	Anderson et al. (1979)	Seawater, 10 to 30 o/oo
Fecal streptococci	18 to 55		Fujioka et al. (1981)	Seawater kept in sunlight
Viruses:				
Coxsackie	0.12 0.03	25 4	Colwell and Hetrick (1975)	Marine waters
Echo 6	0.08 0.03	25 4	Colwell and Hetrick (1975)	Marine waters
Polio type I	0.16 0.05	25 4	Colwell and Hetrick (1975)	Marine waters
Enteric (polio, Echo, and coxsackie)	1.1 to 2.3	24	Fujioka et al. (1980)	Seawater collected off Hawaii

*Range of values or time of year in parenthesis.

sumed to be 2, what percent of fecal coliform bacteria in the downstream discharge should be cut off to meet the standard?

Calculation of fecal coliform bacteria decay rate:

a) the salinity of bathing area

$$S = S_o e^{ux/E} = 7e^{0.01(-5000)/50} = 2.6\,PPT$$

b) the average salinity between the outlet and bathing area

$$\bar{S} = (2.6 + 7.0)/2 = 4.8\,PPT$$

c)Take 35 PPT as 100% sea water salinity, then

$$\%\,seawater = 4.8/35 = 14\ \%$$

d) Decay rate estimation

$$K_b\,(25°C) = [0.8 + (0.006 \cdot 14)]\,1.4 = 1.24\ day^{-1}$$

This decay rate will be used without the calibration or adjustment that is needed in a real problem.

e) Concentration and Bathing Area with no disinfection:

$$N = N_o e^{jx}$$

$$j = \frac{u}{2E}\left(1+\sqrt{1+4EK_B/u^2}\right)$$

$$= \frac{0.01}{2(50)}\left(1+\sqrt{1+4(50)1.24/0.01^2}\right) = 6.4x\,10^{-4}\ 1/m$$

$$N_o = \frac{(4x\,10^6)\,0.5}{200+0.5} = 10^4/100\,ml$$

$$N = 10^4 \cdot e^{6.4x\,10^{-4}(-5000)} = 400/100\,ml$$

Table 5-36. Reported Decay Rate Coefficients for Bacteria and Viruses in Freshwater and Stormwater [Thomann and Mueller (1987), Bowie et al. (1985), and Velz (1984)]

Organism	Dieoff Rate Coefficient (d^{-1} base e)	Temperature (°C)	Reference	Comments
Coliforms:				
Total coliforms	0.8	20	Mancini (1978)	Average freshwater
Total or fecal coliforms	1.2 (summer) 1.1 (winter)	20 5	Frost and Streeter (1924)	From observed disappearance rates in the Ohio River.
	2.0 (Jn/Sept) 2.5 (Oct/May) 0.58 (Dec/Mar) 1.0 (Apr/Nov)	— — — 	Hoskins et al. (1927)	From observed disappearance rates in the Upper Illinois River.
	2.0 (Jn/Sept) 0.9 (Oct/May) 0.62 (Dec/Mar) 0.7 (Apr/Nov)	— — — 	Hoskins et al. (1927)	From observed disappearance rates in the lower Illinois River
	15.1	—	Kittrell and Kochtitzky (1947)	From observed disappearance rates in a shallow turbulent stream
	0.48 (winter)	—	Kittrell and Furfari (1963)	From observed disappearance rates in the Missouri River downstream of Kansas City, Missouri
	1.03 (summer)	—	Kittrell and Furfari (1963)	From observed disappearance rates in the Tennessee River at Knoxville.
	0.12 (summer)	—	Kittrell and Furfari (1963)	From observed disappearance rates in the Tennessee River at Chattanooga.
	1.73 (summer)	—	Kittrell and Furfari (1963)	From observed disappearance rates in the Sacramento River downstream of Sacramento, California
	5.5 (summer)	—	Kittrell and Furfari (1963)	From observed disappearance rates in the Cumberland River in Tennessee.
	2.2 (summer) 1.1 (winter)	—	Velz (1970)	From observed disappearance rates in the Scoito River, Ohio. Original data from Kehr et al.
	1.84 (summer)	—	Velz (1984)	From observed disappearance rates in the Upper Miami River, Ohio. Original data from Velz et al.
	1.84 (summer)	—	Velz (1984)	From observed disappearance rates in the Hudson River,downstream of Albany, New York. Original data from Hall et al.
	26.4		Wasser et al. (1934)	From observed disappearance rates in the Glatt River
	0.5	10	Wuhrmann (1972)	From observed disappearance rates in a groundwater fed stream
	0.41	—	Mahlock (1974)	From observed disappearance rates in the Leaf River, Mississippi
	1.51 (summer)	—	Velz (1984)	From observed disappearance rate in Yaracuy River, Venezula by Parra Pardi.
	0.2 to 0.7	7.9 to 25.5	Klock (1971)	From observed disappearance rates in a wastewater lagoon.
	2.0 1.7	— 19	Marais (1974)	From observed disappearance rates in maturation ponds
	$2.6(1.19)^{T-20}$		Marais (1974)	From observed disappearance rates in oxidation ponds
	8.64	10 to 17	Zanoni et al. (1978)	From observed disappearance rates in Lake Michigan
	9.6 (August)	—	Gannon et al. (1983)	From observed disappearance rates in Ford Lake, Ypsilanti, Michigan
	1.25 2.62 to 0.384 3.3 to 2.7	15 10 20	Thornton et al. (1980)	October 1976, March 1977, June 1977. From observed disappearance rates in DeGray Reservoir, Arkansas.
	1.0	20	Chen et al.	Derived from model calibration(1976)
	0.01 to 3.5	20	Baca and Arnett (1976)	Derived from model calibration for various streams.
	0.48 to 2.0	20	U.S. Army Corps of Engineers (1974)	Derived from model calibration for Lake Ontario.
	0.48	20	Chen and Orlob (1975)	Derived from model calibration for Lake Washington.
	1.0 to 3.0	20	Hydroscience (1971)	Derived from model calibration for various streams.
	0.48	20	Chen and Wells (1975)	Derived from model calibration for Boise River, Idaho.

Table 5-36. Reported Decay Rate Coefficients for Bacteria and Viruses in Freshwater and Stormwater [Thomann and Mueller (1987), Bowie et al. (1985), and Velz (1984)]

Organism	Dieoff Rate Coefficient (d^{-1} base e)	Temperature (°C)	Reference	Comments
Fecal streptococci:				
S.faecalis	0.4 to 0.9	20	USEPA (1974)	Freshwater
	0.1 to 0.4	4		
	0 to 0.8	20	Kenner (1978)	Kanawha River
	0.3	20	Geldrich and Kenner (1969)	Stormwater, observed from 0 to 3rd day
	0.1	20		Observed from 3rd to the 14th day.
	1.0 to 3.0	18	Dutka and Kwan (1980)	Hamilton Bay, Lake Ontario observed from 0 to 10th day.
	0.05 to 0.1			Observed from 10th to 28th day.
S. bovis	1.5	20	Geldrich and Kenner (1969)	Stormwater
Pathogens:				
Salmonella typhinurium	1.1	20	Geldrich and Kenner (1969)	Stormwater, observed from 0 to 3rd day.
	0.1	20		Observed from 3rd to 14th day
Salmonella thompson	0.5 to 3	18	Dutka and Kwan (1980)	Hamilton Bay, Lake Ontario observed from 0 to 10th days
	0.1	18		Observed from 10th to 28th day
Viruses:				
Coxsackie	0.77	21 to 23	Herrmann et al. (1974)	Lake Wingra
Polio type I	0.26	21 to 23	Herrmann et al. (1974)	Lake Wingra
Enteric polio, Echo, and coxsackie)	0.15	0	Dahling and Safferman (1979)	Tanana River, Alaska under ice cover

Fecal Coliform Bacteria Reduction percent with a growth factor of 2

$$\frac{2(400)-200}{2(400)} = 75\%$$

If there is no background concentration of fecal coliform bacteria in the bathing area, reducing the 75% concentration in the fecal coliform bacteria load will result in 200/100 ml fecal coliform bacteria concentration in the bathing area.

SUPPLEMENT VIII: CALIBRATING SIMPLE SEDIMENT MODELS

Section 2.4 and Supplement I of Section 2 introduced the important processes concerning sediment transport in estuaries. Settling is always an important potential factor to water quality problems and a careful analysis and calibration of settling coefficients is always necessary. Limited guidance in the calibration of simple sediment transport models includes:

1. Select initial settling values from Table 5.37 for inorganic particles and Table 5.38 for algae modeling.

2. Adjust settling velocity by trial and error for calibration.

It's important to note that the initial values selected at step 1 do not include the effects of resuspension which can be extremely important to understand the special characteristics of sediment movement in estuaries. During every tidal cycle, particle settling attains a maximum during the slack tides. Later, the sediments on the bottom can be resuspended and carried upstream with flood tide and settle to the bottom there. They can also be carried downstream with ebb flow. For most estuaries, sediments settled onto the bottom layer near the mouth are often carried back into the estuary rather than into the open sea. Usually, at the head of the saline intrusion wedge of a stratified estuary, this upstream transport is balanced by the downstream transport. This point is called the null zone.

In a steady state model a net settling velocity is usually adopted, which equals the gross settling velocity minus resuspension. This net settling can be arrived at by calibrating the model against the suspended solid balance. But, in some situations, this net settling velocity can not be used in describing the pollutant transport. For example, the concentrations of pollutant adsorbed on solids might be appreciably different between the solids settling from the water column and the solids resuspending into the same water due to the sediment movement in the estuary. Also, if a pollutant is newly introduced into an estuary which did not have it before, the gross settling velocity should probably be used to describe the pollutant transport instead of the net settling velocity obtained from the solids balance.

Table 5-37. Settling Velocities in m/day at 20 °C for Inorganic Particles [Ambrose et al. (1987)]

Particle Diameter, mm	Particle Density, g cm^{-3}			
	1.8	2.0	2.5	2.7
Fine Sand				
0.3	300	400	710	800
0.05	94	120	180	200
Silt				
0.05	94	120	180	200
0.02	15	19	28	32
0.01	3.8	4.7	7.1	8.0
0.005	0.94	1.2	1.8	2.0
0.002	0.15	0.19	0.28	0.32
Clay				
0.002	0.15	0.19	0.28	0.32
0.001	0.04	0.05	0.07	0.08

Table 5-38. Settling Velocities for Phytoplankton

Algal Type	Settling Velocity (m/day)	References
Total Phytoplankton	0.05 - 0.5	Chen & Orlob (1975), Tetra Tech (1976), Chen (1970), Chen & Wells (1975,1976)
	0.05 - 0.2	O'Connor et al.(1975,1981) Thomann et al. (1974,1975,1979), Di Toro & Matystik (1980), Di Toro & Connolly (1980), Thomann & Fitzpatrick (1982)
	0.02 - 0.05	Canale et al. (1976)
	0.4	Lombardo (1972)
	0.03 - 0.05	Scavia (1980)
	0.05	Bierman et al. (1980)
	0.2 - 0.25	Youngberg (1977)
	0.04 - 0.6	Jorgensen (1976)
Diatoms	0.05 - 0.4	Bierman (1976), Bierman et al. (1980)
	0.1 - 0.2	Thomann et al. (1979), Di Toro & Connolly (1980)
	0.1 - 0.25	Tetra Tech (1980), Porcella et al. (1983)
	0.03 - 0.05	Canale et al. (1976)
	0.3 - 0.5	Smayda & Boleyn (1965)
	2.5	Lehman et al. (1975)
Green Algae	0.05 - 0.19	Jorgensen et al. (1978)
	0.05 - 0.4	Bierman (1976), Bierman et al. (1980)
	0.02	Canale et al. (1976)
	0.8	Lehman et al. (1975)
	0.1 - 0.25	Tetra Tech (1980), Porcella et al. (1983)
	0.3	DePinto et al. (1976)
Blue-green Algae	0.05 - 0.15	Bierman (1976), Bierman et al. (1980)
	0.	Canale et al. (1976)
	0.2	Lehman et al. (1975)
	0.1	DePinto et al. (1976)
	0.08 - 0.2	Tetra Tech (1980), Porcella et al. (1983)
Flagellates	0.5	Lehman et al. (1975)
	0.05	Bierman et al. (1980)
	0.09 - 0.2	Tetra Tech (1980), Porcella et al. (1983)
Dinoflagellates	8.0	O'Connor et al. (1981)
Chrysophytes	0.5	Lehman et al. (1975)
Coccolithophores	0.25 - 13.6	Collins & Wlosinski (1983)

SUPPLEMENT IX: SELECTION OF CBOD COEFFICIENTS

Carbonaceous biochemical oxygen demand (CBOD) is the utilization of oxygen by aquatic microorganisms to metabolize organic matter and the oxidation of any reduced minerals such as ferrous iron, methane, and hydrogen sulfide that may leach out or be transported from the anaerobic layers in bottom sediments. In addition, there are usually significant amounts of unoxidized nitrogen in the form of ammonia and organic nitrogen that must be taken into account. To improve the chances for describing the oxygen balance, however, nitrogenous BOD (NBOD) is generally simulated separately as will be discussed in Supplement VIII. The total effect of CBOD and NBOD has been modeled on occasion as total BOD (= CBOD + NBOD) but this is not recommended for waste load allocations because of the difficulty in forecasting total BOD. Occasionally, total BOD is used in screening-level models where adequate data are not available, but these types of studies should not be confused with a more precise waste load allocation model study. Figure 5.28 shows the major sources and sinks of CBOD in surface waters including estuaries. Point sources are usually the most important source of CBOD and because these are the most controllable sources, they are typically the focus of the waste load allocation. However, nonpoint sources, autochthonous sources due to the recycling of organic carbon in dead organisms and excreted materials, the benthic release of reduced minerals and

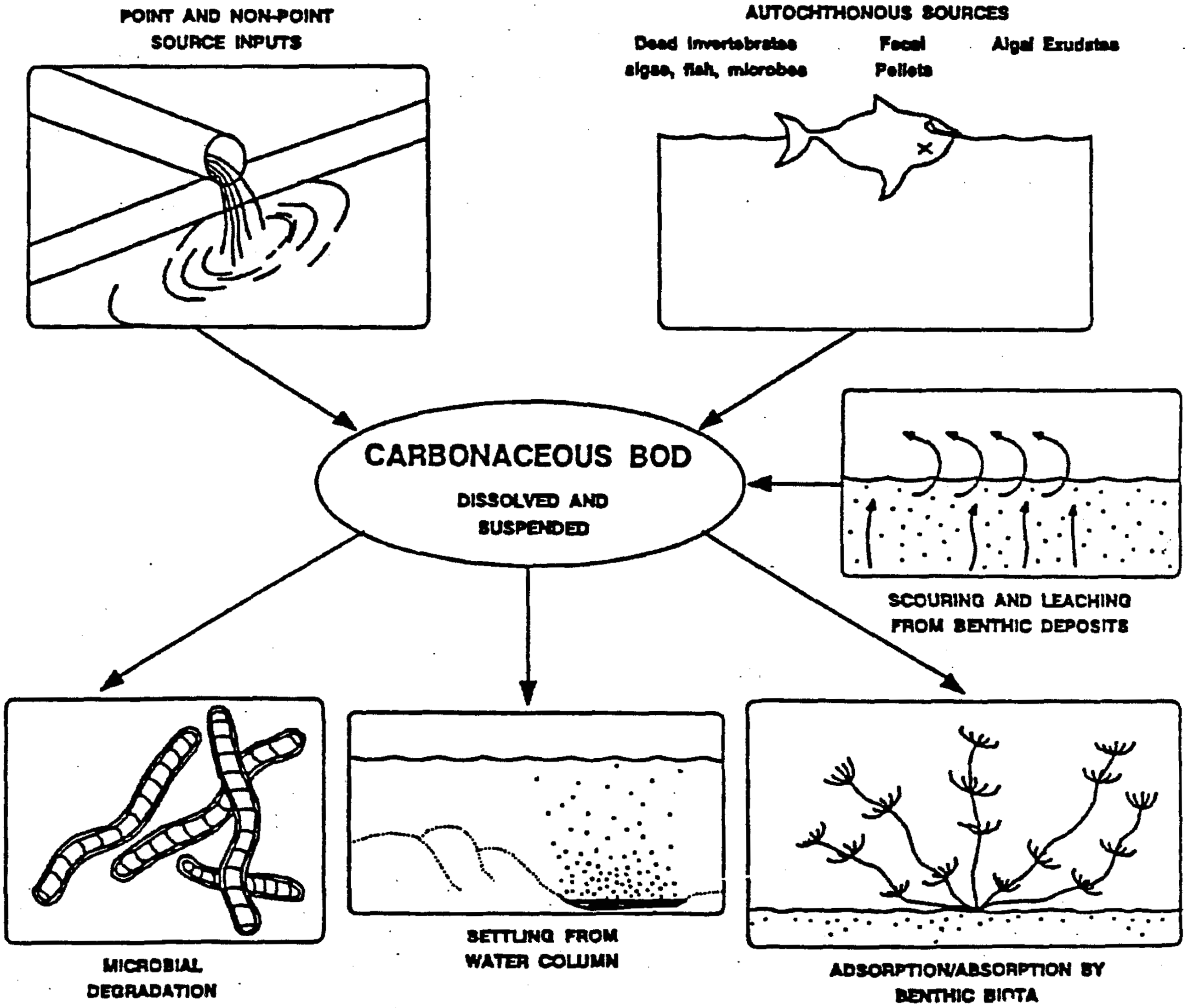


Figure 5-28. Sources and sinks of carbonaceous BOD in the aquatic environment [Bowie et al. (1985)].

scour and leaching of organic carbon, can be quite important as well. In fact, many point sources already have been controlled to the point that any further improvements in water quality may require waste load allocation of the diffuse and less readily controlled nonpoint sources. For example, the continued anoxia in Chesapeake Bay seems to indicate as much. In any event, it is important that background sources of CBOD be adequately quantified to determine the relative importance compared to point sources. If other sources are relatively important, they too must be included in the CBOD mass balance or the calibrated model will be inadequate for aiding waste load allocation.

CBOD is removed from the water column by three processes. First, carbonaceous material is oxidized by microbes causing a reduction in CBOD. Typically, this is the dominant process that must be taken into account. Second, CBOD can settle out of the water column. This occurs in two ways. Particulates immediately begin to settle unless sufficient turbulence is present to maintain the suspension. This is aided by the tendency of saline water to stabilize freshwater particulates and assist in flocculation and increased settling. In addition, dissolved CBOD can be adsorbed and assimilated by bacteria cell synthesis without immediate oxidation. These bacteria also can settle, especially as part of any floc generated as a result of the stabilization of freshwater particles. Third, dissolved CBOD can be adsorbed by benthic biota, especially by filamentous growth on surfaces, and benthic plants can filter particulate material. However, there is usually limited contact between benthic bacteria and plants, and the water column with the result that only oxidation and, occasionally, settling are the important processes to describe in calibrating a model. Exceptions to the general expectations occur when significant interactions occur with tidal flats and adjoining wetlands. Also in brackish and saline waters, metabolism is slower (Krenkel and Novotny 1980) compared to freshwater so there is also less of a tendency for organic carbon to be assimilated for cell synthesis. As a result, the CBOD mass balance is usually quite simple except near the outfall and at the interface or mixing zone between saline and freshwater where settling is more likely. In general, the CBOD mass balance is expressed as:

$$\frac{dL}{dt} = -K_r L + L_a \qquad (5.30)$$

where L is ultimate CBOD in mg L^{-1}, t is time, K_r is the first order rate constant describing the reduction in CBOD, and L_a is the zero order CBOD resuspension or reentrainment rate in mg L^{-1} d^{-1}. K_d is actually a combination of the coefficient for oxidation, settling and adsorption:

$$K_r = K_d + K_s + K_u \qquad (5.31)$$

where K_d is the water column deoxygenation rate coefficient (i.e., oxidation rate) in d^{-1}, K_s is the settling rate coefficient in d^{-1}, and K_u is the sorption rate coefficient in d^{-1}. Unexplainable discrepancies occasionally are observed (see Krenkel and Novotny 1980), but in general, K_d can be estimated from the bottle deoxygenation rate coefficient, K_1, determined from long term CBOD tests (see Whittemore et al. 1989, Stamer et al. 1979, or McCutcheon et al. 1985 for a description of the test and data analysis procedures). This seems to be especially true for samples collected from larger bodies of water like large rivers (Mackenzie et al. 1979), lakes, and estuaries where suspended bacteria are more important than attached bacteria in oxidizing organic matter and the samples are not diluted. K_s can be estimated from settling velocity tests like those involving the Imhoff cone (Standard Methods 1985), where

$$K_s = \frac{V_s}{D} \qquad (5.32)$$

V_s is the settling velocity measured in m d^{-1} and D is depth of flow in m. Unfortunately, Equation (5.32) is only useful in describing the settling of discrete particles. When flocculation or disaggregation occurs, V_s typically changes by orders of magnitude at times. At present, the effect of flocculation and disaggregation can not be described. As a result, K_s can not be readily estimated. In addition, K_u can not be readily estimated for typical field studies. Therefore, a calibration parameter, $K_3 = K_s + K_u$, is defined and selected by trial and error. Generally, it is possible to locate large areas where $K_3 = 0$ so that K_d can be selected. If K_d is not approximately equal to the bottle coefficient, K_1, additional investigation is required to re-evaluate K_d and determine whether the initial calibration value may actually be $K_d + K_s + K_u$. Once K_d is properly selected, K_3 can be determined in other parts of the estuary where settling and sorption are occurring by selecting $K_d + K_3$ so that model predictions agree with measurements. Likewise, L_a can be determined in other areas where re-entrainment of organic materials or leaching of reduced materials occur. Typically, scour of organic particles is expected when velocities near the bed exceed 0.2 to 0.3 m s^{-1} (0.6 to 1 ft s^{-1}). Any zones with high near bed velocities approaching these velocities should be investigated. Because estuaries are normally a net depositional regime, however, L_a can probably be ignored as a first approximation unless extensive organic deposits are evident (e.g., like the tidally affected reaches of the Willamette River where recent uncontrolled point source discharges of wood fibers caused long-lasting organic deposits). Therefore, sludge and organic deposits should be mapped if possible to show where L_a may exceed zero.

SUPPLEMENT X: SELECTION OF NBOD COEFICIENTS

There are two usual approaches to describe the transformation of oxidizable nitrogen. One is to consider the actual process of transformation: from organic nitrogen, through nitrite to nitrate, where oxygen consumption is involved in the process. This will be discussed in Supplement XI. The other approach that will be discussed here simply lumps the organic and ammonia nitrogen together (called total kjeldahl nitrogen, TKN). This total kjeldahl nitrogen will be oxidized through a first-order decay. The oxidation of TKN is NBOD.

Decay of NBOD is written as

$$dt = \frac{dN}{-K_N N} \tag{5.33}$$

Where

N = NBOD concentrations, mg/L.

NBOD = $4.57(N_o + N_i) + 1.14N_2$ can be used as the upper limit of NBOD (see Bowie et al. 1985)

N_o = organic nitrogen concentrations, mg/L

N_i = ammonia nitrogen concentration, mg/L

N_2 = nitrite-nitrogen concentration, mg/L

K_N = overall NBOD reaction rate, 1/day

According to Thomann and Mueller (1987), the range of K_N values is close to the deoxygenation rate of CBOD, and for large water bodies, the typical range is 0.1-0.5/day at 20°c; but for small streams, it can often be expected to be greater than 1/day. Table 5.39 compiles the available first-order NBOD decay rates in estuaries that can be helpful in selecting initial NBOD decay rates. The effects of temperature on K_N can be estimated by

$$(K_N)_T = (K_N)_{20} \cdot 1.08^{T-20} \tag{5-34}$$

for $10 < T < 30°C$

Where 1.08 = average temperature correction coefficient (see Bowie et al. 1985)

When temperature goes higher than 30°C, the nitrification rate is inhibited by the high temperature and the relationship is no longer valid. When temperature is below 10°C, the nitrifying bacteria do not multiply very well and the above equation will give a K_N that is too high. So, when temperature is below 5-10°C, K_N is usually set to zero (Thomann and Mueller 1987).

pH is also an important factor to the nitrification rate (Bowie et al. 1985). The optimal pH for nitrification is about 8.5. When pH is outside the range of 7.0 to 9.8, the nitrification rate can be reduced significantly. If pH is lower than 6.0, no nitrification is expected.

Table 5-39. First-Order Nitrification Rate Constants Observed in Estuaries (constants are in d^{-1}) [Bowie et al. (1985)]

Estuary	Maximum	Average	Minimum	Reference	Comment
Potomac	0.14	–	0.10	Slayton and Trovato (1978, 1979)	Measured by BOD bottle tests; data fit with Thomas Graphical Method
Potomac	–	0.09 to 0.13	–	Thomann and Fitzpatrick (1982)	Derived from model calibration
Delaware	0.54	0.3	0.09	Bansal (1976)	
New York Bight	–	0.09	–	O'Connor et al. (1981)	

Table 5-40. Rate Coefficients for Nitrogen Transformations [Bowie et al. (1985)]
(K = 1st order rate coefficient in d^{-1} and θ = temperature correction factor)

PON[a]→DON		DON→NH3		PON→NH3		NH3→NO2		NH3→NO3		NO2→NO3		SEDN→NH3		References
K	θ	K	θ	K	θ	K	θ	K	θ	K	θ	K	θ	
Calibration values derived from field data														
				0.035	linear			0.04	linear					Thomann et al. (1976)
				0.03[b]	1.08									Thomann et al. (1979)
				0.03[c]	1.08			0.12[b]	1.08			0.0025	1.08	DiToro and Conolly (1980)
				0.03[c]	1.08			0.20	1.08					DiToro and Matystik (1980)
				0.075	1.08			0.09-0.13[c]	1.08			0.004	1.08	Thomann & Fitzpatrick (1982)
								0.025[c]	1.08					O'Connor et al. (1981)
				0.14	linear									Salas and Thomann (1973)
				0.001	1.02	0.003-0.03	1.02			0.09	1.02	0.001	1.02	Chen & Orlob (1972, 1975)
0.020	linear	0.020	linear					0.060	linear					Scavia et al. (1976)
0.020	linear	0.020	linear					0.1	linear					Scavia (1980)
0.02	1.020	0.02	1.020					0.1	1.020					Bowie et al. (1980)
0.02	linear	0.024	linear					0.16	linear					Canale et al. (1976)
				0.003	1.020	0.02	1.047			0.25	1.047	.0015	1.047	Tetra Tech (1980)
				0.1	1.047	0.02	1.047			0.25	1.047	.0015	1.047	Porcella et al. (1983)
				0.01[b]	NI							0.95-1.8[c]	1.14	Nyholm (1978)
				.005[b]	1.08									Bierman et al. (1980)
				0.1[b]	1.02									Jorgensen (1976)
				0.2[b]	1.072									Jorgensen et al. (1978)
Recommendations from Model Documentation														
				.1-.4	NI	.1-.5	NI			5.-10.	NI			Baca et al. (1973)
				0.02-0.04	1.02-1.09	.1-.5	1.02-1.09			3.-10.	1.02-1.09	.01-.1	1.02-1.09	Baca and Arnett (1976)
						.1-.5	1.047			0.5-2.0	1.047			Duke and Marsh (1973)
						.1-.5	1.047			0.5-2.0	1.047			Roesner et al. (1978)
				.005-.05	1.02-1.04	.05-.2	1.02-1.03			0.2-0.5	1.02-1.03	.001-.01	1.02-1.04	Smith (1979)
				.001-.02	1.045	.05-.2	1.02			0.2-0.5	1.02	.001-.02	1.040	Brandes (1976)
								0.04-3.0	logistic					Granney and Krassenski (1981)
								0.001-1.3[d]	NI					Collins and Wlosinski (1983)

[a] Abbreviations are defined as follows:
NI - no information
PON - Particulate Organic Nitrogen
DON - Dissolved Organic Nitrogen
SEDN - Sediment Organic Nitrogen
Linear refers to linear temperature correction.
Logistic refers to logistic theory of growth parameters.

[b] Unavailable nitrogen decaying to algal-available nitrogen.

[c] DiToro & Connolly (1980) & Di Toro & Matystik (1980) multiply the PON-NH_3 rate by a chlorophyll limitation factor, Chl a/K_1 + Chl a, where K_1 is a half-saturation constant = 5.0 mg Chl a/L.
DiToro & Connoly (1980) and Thomann & Fitzpatrick (1982) multiply the NH_3-NO_3 rate by an oxygen limitation factor, $O_2/K_2 + O_2$, where K_2 is a half-saturation constant = 2.0 mg O_2/L.
O'Connor et al. (1981) multiply the NH_3-NO_3 rate by an oxygen limitation factor, $O_2/K_3 + O_2$, where K_3 is a half-saturation constant = 0.5 mg O_2/L.
Nyholm (1978) used a sediment release constant which is multiplied by the total sedimentation rate of algae and detritus.

[d] Literature value.

The nitrogen cycle plays an important role in water quality problems through its biochemical effects and oxygen consumption. Table 5.40 compiles the available values of rate coefficients for some important nitrogen transformations, including ammonification and nitrification. The coefficients for ammonification, which means the release of ammonia due to the decay of organic nitrogen in the water column and sediments, are very site dependent and not as well documented as the coefficients of nitrification, which means the oxidation of ammonia through nitrite to nitrate consuming dissolved oxygen at the same time.

Table 5.41 lists the coefficients for the denitrification process which reduce the nitrate of N_2 under anaerobic conditions.

Values in the above two tables can be used as a guidance for selecting initial values of these coefficients. Models should be calibrated for the specific problem later on.

Table 5-41. Rate Coefficients for Denitrification [Bowie et al. (1985)]

Nitrate → Nitrogen Gas		
K	θ	References
0.1*	1.045	Di Toro and Connolly (1980)
0.1**	1.045	Di Toro and Connolly (1980)
0.09*	1.045	Thomann and Fitzpatrick (1982)
0.1*	1.045	O'Connor et al. (1981)
0.002	No information	Jorgensen (1976)
0.02-0.03	No information	Jorgensen et al. (1978)
0.0-1.0***	1.02-1.09***	Baca and Arnett (1976)

*This rate is multiplied by an oxygen limitation factor, $K_1/[K_1+O_2]$, where K_1 is a half-saturation constant = 0.1 mg O_2/L

** The same rate applies to sediment NO_3 denitirfication

*** Model documentation values

Another important phenomenon that needs to be mentioned is the toxity of un-ionized ammonia to aquatic life. The ionization equibrum is

$$NH_3 \cdot nH_2O \rightleftharpoons NH_4^+ + OH^- + (n-1) \cdot H_2O \quad (5.35)$$

Equibrum is reached rapidly, and is largely controlled by pH and temperature. Figure 5.29 gives the percentage of un-ionized ammonia under different pH and temperature conditions. Usually, water quality models predict ammonium concentration, which can be related to the total concentration in Fig. 5.29. Additional guidance on processes affecting ammonia toxicity may be found in U.S. EPA (1985b and 1989).

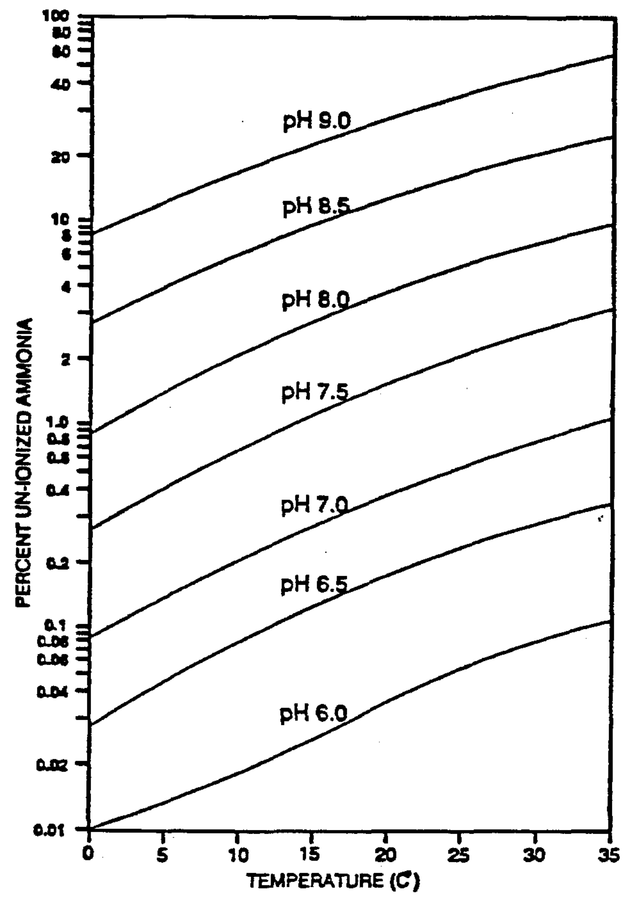


Figure 5-29. Effect of pH and temperature on un-ionized ammonia [Willingham (1976)].

SUPPLEMENT XII: PHOSPHORUS CYCLE COEFFICIENTS

Guidance on the selection of phosphorus cycle model coefficients is given in Table 5.42.

Table 5-42. Rate Coefficients for Phosphorus Transformations [Bowie et al. (1985)]
(K = 1st order rate coefficient in d^{-1} and θ = temperature correction factor)

POP→DOP		POP→PO4		DOP→PO4		SEDP→DOP		SEDP→PO4		References
K	θ	K	θ	K	q	K	θ	K	θ	
		0.14	linear							Thomann et al. (1975)
		0.03	1.08							Thomann et al. (1975)
		0.03[b]	1.08							DiToro and Conolly (1980) DiToro and Matysik (1980) Salsbury et al. (1983)
0.22[b]	1.08			0.22[b]	1.08	0.0004	1.08	0.0004	1.08	Thomann & Fitzpatrick (1982)
		0.14	linear							Salas and Thomann (1978)
		0.001	1.02					0.001	1.02	Chen & Orlob (1972, 1976)
		0.02	linear							Scavia et al. (1976) Scavia (1980)
0.22[b]	linear									Connie et al. (1976)
		0.003	1.020					0.0015	1.047	Tetra Tech (1980)
		0.02	1.020					0.001	1.020	Bowie et al. (1980)
		0.1	1.047					0.0015	1.047	Porcalia et al. (1983)
		0.1	1.14					1.04147	1.14[b]	Nyholm (1978)
		0.005	1.08							Bierman et al. (1980)
		0.1	1.02					0.0018	1.02	Jorgensen (1976)
		0.5-0.6	1.072							Jorgensen et al. (1978)
		0.1-0.7[c]	1.02-1.09[c]					0.1-0.7[c]	1.02-1.09[c]	Baca et al. (1973)
		0.1-0.7[c]	1.02-1.09[c]							Baca and Arnett (1976)
		0.005-0.05[c]	1.02-1.04[c]					0.004-0.04[c]	1.02-1.04[c]	Smith (1976)
		0.001-0.02[c]	1.040[c]							Brandes (1976)

Sediment						References
DOP→PO4		SA→DOP		SA→PO4		
K	θ	K	θ	K	θ	
0.0004	1.08	0.02	1.08	0.02	1.08	Thomann & Fitzpatrick (1982)

Abbreviations are defined as follows:
- POP - Particulate Organic Phosphorus
- DOP - Dissolved Organic Phosphorus
- SEDP - Sediment Organic Phosphorus
- PO4 - Phosphate
- SA - Settled Algae
- Linear - linear temperature correction assumed.

[b] DiToro & Connolly (1980), DiToro & Matystik(1980) and Salsibury et al. (1980) multiply this rate by a chlorophyll limitation factor, Chl a/K_1 + Chl a, where K_1 is a half-saturation constant = 5.0 mg Chl a/L. Thomann & Fitzpatrick (1982) multiply this rate by an algal carbon limitation factor, Algal-C/K_2+Algal-C, where K_2 is a half-saturation constant = 1.0 mg C/L. Nyholm (1978) uses a sediment release constant which is multiplied by the total sedimentation of algae and detrirus.

[c] Model documentation values.

SUPPLEMENT XIII: SELECTION OF REAERATION COEFFICIENTS

Three methods are used to select reaeration coefficients:

1. Reaeration coefficients are computed by various empirical and semi-empirical equations that relate K_2 to water velocity, depth, wind speed and other characteristics of the estuary.

2. Reaeration occasionally is determined by calibration of the model involved.

3. Reaeration is measured using tracer techniques on rare occasions.

In most cases, K_2 is computed by a formula that is included in the model being applied. Only a very few models (see Bowie et al. 1985 for example) force the user to specify values of K_2, the reaeration rate coefficient, or K_L, the surface mass transfer coefficient. Also infrequently applied, but expected to be of increasing importance, is the measurement of gas transfer.

Whether a study should concentrate on estimation of K_2 or K_L depends on the nature of the flow. When water surface turbulence is caused by bottom shear and the flow is vertically unstratified, formulations for K_2, similar

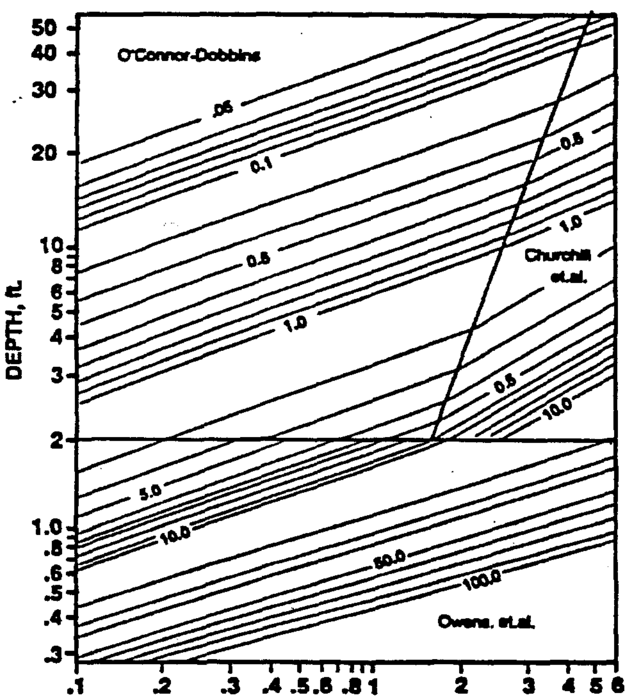


Figure 5-30. Reaeration Coefficient (day^{-1} versus depth and velocity using the suggested method of Covar (1976) [Bowie et al. (1985)].

to those used in streams are the most useful. When the flow is vertically stratified and wind shear dominates water turbulence at the surface, K_L is typically specified. The values of K_2 and K_L are related according to:

$$K_2 = \frac{K_L}{H} \tag{5.36}$$

where H is the average depth with the units of meters when K_L is expressed in units of m d^{-1}. In effect, K_2 is the depth-averaged value of K_L when the depth is equal to the volume of the water body or segment divided by the area of the water surface.

When reaeration is dominated by the shear of flow on the bottom boundary, the O'Connor-Dobbins equation (see O'Connor and Dobbins 1958, Table 5.43) has been used almost exclusively to estimate K_2. The reason for this is that the equation is derived from the film penetration theory, which seems to be applicable for most of the conditions found in estuaries except those related to wind-generated turbulence (i.e. flows are deep to moderately deep and rarely very shallow, and velocities range from zero to moderately fast but never extremely fast). Covar (1976) defines, in more precise terms, what are thought to be the limitations of the O'Connor-Dobbins equation. Generally, flows should be deeper than approximately 0.6 m (2 ft) and velocities should not exceed 0.5 m s^{-1} (1.5 ft s^{-1}) at depths of 0.6 m (2 ft) or exceed 1.5 m s^{-1} (5 ft s^{-1}) at depths of 15 m (50 ft) as illustrated in Figure 5.30. Estimation errors are expected to be small, however, if velocities only occasionally exceed 0.5 m s^{-1} to 1.5 m s^{-1} (1.5 ft s^{-1} to 5 ft s^{-1}) as noted in Figure 5.30.

If alternative formulations seem necessary, it may be useful to examine those in Table 5.43. Following the O'Connor-Dobbins equation, the Hirsh equation (McCutcheon and Jennings 1981), the Dobbins equation, and the Churchill et al. equations may be most useful. The Hirsh equation is derived from the Velz iterative method using the surface renewal theory that has been used extensively in estuaries and deeper streams. Experience indicates that this equation may be most appropriate for deeper, stagnant bodies of water that are more sheltered. This equation seems to provide a minimum estimate of K_2 not related to velocity. Alternatively, expert practitioners (personal communication, Thomas Barnwell, Jr., U.S. EPA Center for Exposure Assessment Modeling) use a minimum estimate on the order of 0.6/D where depth is in meters. The equations by Churchill et al. (1962) are included because of the applicability at higher velocities in deeper flows. The complex equation by Dobbins is

Table 5-43. Formulas to Estimate Reaeration Coefficients for Deeper, Bottom Boundary Generated Shear Flows [Bowie et al. (1985), Rathbun (1977), Gromiec et al. (1983), and McCutcheon (1989)]

Citation	K2 (base e, 20°C, day^{-1})	Units	Applicability
Derived from Conceptual Models			
O'Connor and Dobbins (1958)	$\frac{12.8u^{1/2}}{D^{1.5}}$	U: ft/s D: ft U:m/s D:m	Conceptual model based on the film penetration theory for moderately deep to deep rivers; 1 ft≤D≤30 ft (0.3 m≤D≤9.1 m), 0.5 ft/s≤U≤1.6 ft/s (0.15 m/s≤U≤0.49 m/s), 0.005/d≤K_2≤ 12.2/d. O'Connor and Dobbins developed a second formula but O'Connor (1960) noted that the difference between the two formulas was insignificant and recommended the use of this form.
Dobbins (1964)	$\frac{C_1[1+F^2(US)^{0.375}]}{(0.9+F)^{1.5}D} \coth\left[\frac{4.10(US)^{0.125}}{(0.9+F)^{0.5}}\right]$ coth [ ] is the hyperbolic contangent	for C_1 = 117 U:ft /s D:ft S:ft/ft for C_1 = 62.4 U:m/s D:m S:m/m	Based on film penetration model combined with data from natural streams and the flume data of Krenkel and Orlob (1963)
Semi-Empirical Models			
Krenkel and Orlob (1962, 1963)	$\frac{C_2(US)^{0.408}}{D^{0.660}}$ or $\frac{8.4(D_x)^{1.321}}{D^{2.32}}$ or $\frac{0.0024(D_x)^{1.321}}{D^{2.32}}$ $\frac{2.6(D_y)^{1.237}}{D^{2.087}}$	C_2 = 234 U:ft/s S:ft/ft D:ft C_2 = 174 U:m/s D:m S:m/m D_x:ft^2/s D:ft D_x:m^2/min D:m D_y:m^2/s D:m	Energy dissipation model calibrated by multiple correlation analysis using 1-ft (0.3-m) wide flume data; 0.08 ft≤D≤0.2 ft (0.02 m≤D≤0.06 m). Based on correlation with longitudinal and vertical disperson and calibration with data from 1-ft (0.3-m) wide flume with deoxygenated water. Other similar forms were also reported. The flume D_x was less than that typically encountered in streams.
Thackston and Krenkel (1969)	$\frac{C_3(1+F^{1/2})u^*}{D}$ or A_4Q^B, where A_4 and B = constants	C_3 = 24.9 u*:ft/s D:ft C_3 = 24.9 u*:m/s D:m	Calibrated with measurements of deoxygenated water in a 2-ft (0.61-m) wide flume; 0.05 ft≤D≤ 0.23 ft (0.015 m≤D≤0.091 m). Derived from the original equation given above.
Tivoglou and Wallace (1972)	(4700)US or 0.054(Δh/Δt) at 25°C (15,300)US or 0.18(Δh/Δt) at 25°C	U:ft/s S:ft/ft Δh:ft Δt:d U:m/s S:m/m Δh:m Δt:d	Energy dissipation model calibrated from radioactive tracer measurements in five rivers.

Table 5-43. Formulas to Estimate Reaeration Coefficients for Deeper, Bottom Boundary Generated Shear Flows [Bowie et al. (1985), Rathbun (1977), Gromiec et al. (1983), and McCutcheon (1989)] (concluded)

Citation	K2 (base e, 20°C, day^{-1})	Units	Applicability
Semi-Empricial Models (continued)			
McCutcheon and Jennings (1982)	$\dfrac{-\ln\left[1-2\left(\dfrac{D_m I \; 24}{\pi(30.48D)^2}\right)^{1/2}\right]}{I}$ $D_m = 1.42(1.1)^{T-20}$ $[I = 0.0016+0.0005\,D\,]\; D \le 2.26$ ft $[I = 0.0097\ln(D) - 0.0052]\; D > 2.26$ ft	D:ft T:°C	Originally derived by Hirsch (1972) to replace the Velz (1984) interative method. Expressions for the mix interval, I are derived from the extensive experience in applying the interative method. The underlying concept is similar to the surface-renewal theory.
Churchill et al. (1962)	$\dfrac{0.035U^{2.695}}{D^{3.085}S^{0.823}}$ $\dfrac{0.746U^{2.695}}{D^{3.085}S^{0.823}}$	U:ft/s D:ft U:m/s D:m	Based on dimensional analysis. Derived from data collected in rivers below Tennessee Valley Authority (U.S.) dams.
Empirical Formulas			
Churchill et al. (1962)	$\dfrac{11.6U^{0.969}}{D^{1.673}}$ $\dfrac{5.01U^{0.969}}{D^{1.673}}$ or $\dfrac{6.91U}{D^{1.67}}$	U:ft/s D:ft U:m/s D:m	See Churchill et al. above. This form almost as good and is recommended by Churchill et al. 2 ft(0.61 m)≤D≤11 ft (3.35 m) and 1.8 ft/s≤U≤5 ft/s (0.55 m/s≤U≤1.5 m/s)
Owens et al. (1964)	$\dfrac{21.7U^{0.67}}{D^{1.85}}$ $\dfrac{5.32U^{0.67}}{D^{1.85}}$	U:ft/s D:ft U:m/s D:m	Developed from oxygen recovery data collected on six English streams following deoxygenation with sodium sulfide by Gameson et al. (1955) and Owens et al. (1964) and collected below TVA dams by Churchhill et al. (1962); 0.1 ft/s≤U ≤5 ft/s (0.03 m/s≤U≤1.5 m/s).
Owens et al. (1964)	$\dfrac{23.3U^{0.73}}{D^{1.75}}$ $\dfrac{6.92U^{0.73}}{D^{1.75}}$	U:ft/s D:ft U:m/s D:m	This second formula was developed for 0.1 ft/s ≤U≤1.8 ft/s (0.03 m/s≤U≤0.55 m/s); 0.4 ft≤ D≤1.5 ft (0.12 m≤D≤0.46 m) from a restricted data set at the Water Pollution Research Laboratory.
Harleman et al. (1977)	$10.86\dfrac{U^{0.6}DW}{D^{1.4}A}$	U:ft/s D:ft W:ft A:ft^2	Equation of unknown original developed for the MIT Transient Water Quality Model.
Ozturk	$4.56\dfrac{U^{4/3}}{D}$	U:m/s D:m	Equation developed exclusively for estuaries. See Bowie et al. (1985)

Notation:

U = averaged velocity or tidal velocity [Harleman (1977)]
D = average depth of flow.
F = $U/(gD)^{1/2}$ = Froude number.
g = gravitational constant.
S = slope of water surface.
D_x = longitudinal dispersion coefficient.
D_y = averaged vertical eddy diffusivity.
u_* = $(gDS)^{1/2}$ = shear velocity.
Q = stream discharge.
h = change in water surface elevation in a reach (between two points).
t = time of travel in the reach over which change in elevation is measured.
D_m = molecular diffusion coefficient for oxygen in water.
T = water temperature
I = mix interval.
W = top width of estuary.
A = cross sectional area.

Table 5-44. Constant Values of Surface Mass Transfer Coefficients Applied in the Modeling of Estuaries, Coastal Waters, and Lakes [Bowie et al. (1985)]

KL (m d-1)	Location or type of water body	Reference	Comment
1	New York Bught	O'Connor et al. (1981)	
0.6	Estuaries	O'Connor (personal communication)	
2	Lake Erie	Di Toro and Connolly (1980)	
0.1	Confined disposal in lakes	Martin et al. (1989)	Crude estimate for diked facilities in the Great lakes
0.4	Lakes	Weiler (1975)	See Bowie et al. (1985)

Table 5-45. Empirical Wind Speed Relationships for Mass Transfer and Reaeration Coefficients [Bowie et al. (1985)]

Reference	Formulation	Comment
	Estuaries	
Thomann and Fitzpatrick (1982)	$K_2 = 13\frac{U^{0.5}}{D^{1.5}} + \frac{3.281}{D}(0.728u^{0.5} - 0.371u + 0.0372u^2)$ K2 in d-1, D in ft, U in ft s-1, u in m s-1	Applied in the Potomac Estuary. Combines O'Connor-Dobbins and wind speed formulations.
	Lakes	
Chen et al. (1976)	$K_L = \frac{86{,}400 D_m}{(200-60u^{0.5})\times 10^{-6}}$ Dm in m2s-1, u in m s-1	
Banks (1975)	$K_L = 0.362u^{1/2}$ for $0 < u < 5.5$ m s -1 $K_L = 0.0277u^2$ for $u > 5.5$ m s -1	

Notation:

K_2 = reaeration coefficient (T^{-1}),
K_L = surface mass transfer coefficient ($L\,T^{-1}$),
U = depth averaged velocity ($L\,T^{-1}$),
D = Depth (L),
u = wind speed ($L\,T^{-1}$),
D_m = molecular diffusion coefficient for oxygen in water ($L^2\,T^{-1}$),
a = empirical coefficient, and
b = empirical coefficient.

included because its rational derivation indicates that it may be occasionally useful. The Krenkel and Orlob (1962) and Thackston and Krenkel (1969) energy dissipation equations are included for similar reasons, although these equations are more applicable to shallower depths than the Dobbins equation. The equation by Ozturk (1979) is included for completeness but little is known about the limitations of applicability and usefulness. Finally, the Tsivoglou and Wallace (1972) energy dissipation equation is included because it is now widely thought to be the best method for predicting K_2 in shallow turbulent flows in place of the Owens et al. (1964) equation given in Figure 5.30 from Covar (1976). When estimated K_2 values are too small, maximum velocities observed during the tidal cycle or the average of the absolute velocity are used in place of tidal or average velocities in the O'Connor-Dobbins (1958) and other velocity type equations [i.e. Harleman et al. (1977)].

If the estuary is dominated by bottom-shear-generated turbulence, selection of K_2 values seems to best be guided as follows:

1) Compute K_2 from the O'Connor-Dobbins equation (see Table 5.43 for the equation).

2) Check to be sure that K_2 exceeds or equals a minimum value of approximately 0.6/depth.

3) If K_2 seems to be over-predicted, investigate use of the Hirsh equation (see Table 5.43 for the equation).

4) If K_2 seems to be under-predicted, investigate the use of the maximum tidal velocity or the tidally averaged absolute velocity or determine if wind shear may be important.

5) To investigate the importance of wind shear, compute K_L from the screening level equations of Kim and Holley (1988), divide by the depth and compare with values computed by the O'Connor-Dobbins equation. If wind shear does seem important, compute K_L values from the O'Connor (1983) formulations.

When estuarine reaeration is dominated by wind-generated water turbulence, or the flow is deep and stratified, two approaches have been found to be useful. First, many studies in open coastal waters and lakes specify a constant value of K_L. Table 5.44 lists some of the known examples. Second, there are a number of semi-empirical and empirical formula relating K_2 or K_L to wind speed measurements. These are listed in Table 5.45.

The selection of K_L values seem to be best made according to the following procedure:

1) Select a constant K_L, especially if surface dissolved oxygen is near saturation (Bowie et al. 1985, Di Toro and Connolly 1980) and test to see if this adequately closes the dissolved oxygen balance in the model employed.

2) If the dissolved oxygen balance is not adequately closed, compute K_L according to the method of O'Connor (1983).

3) If K_L values still do not seem to be correct, determine whether any of the other wind speed relationships in Table 5.33 are useful. The crude screening approach of Kim and Holley (1988) may be the next most useful approach

SUPPLEMENT XIV: PROGRAM OF O'CONNOR'S METHOD TO COMPUTE K_2 IN WIND DOMINATED ESTUARIES

D.J. O'Connor, (1983) developed a relation between the transfer coefficient of slightly soluble gases (i.e. reaeration coefficient, K_L for oxygen) and wind velocity. This method assumes that reaeration is a wind dominated process. The functions relating the viscous sublayer and roughness height with the wind shear provide the basis for the development of equations which define the transfer coefficient.

For hydrodynamically smooth flow, viscous conditions prevail in the liquid sublayer which controls transfer and the transfer is effected solely by molecular diffusion. In fully established rough flow, turbulence extends to the surface and turbulent transfer processes dominant. In the transition region between smooth and rough flow where both transfer mechanisms contribute, O'Connor envisions the exchange as a transfer in series and the overall coefficient ($1/K_L$) described by

$$\frac{1}{K_L} = \frac{1}{K_z} + \frac{1}{K_r} \qquad (5.37)$$

where K_r is the transfer coefficient through the diffusional sublayer and K_z is the surface renewal transfer at the boundary of the diffusional sublayer.

Based on the physical behavior in the smooth and rough layers K_L is then developed by O'Connor as

$$\frac{1}{K_L} = \frac{1}{\left[\frac{D}{\nu_w}\right]^{2/3} \frac{\kappa^{1/3}}{\Gamma(u_*)} \frac{\rho_a u_*}{\rho_w}} + \frac{1}{\left[\frac{D u_*}{\kappa z_0 u_*} \frac{\rho_a \nu_a}{\rho_w \nu_w}\right]^{1/2}}$$

(5.38)

where

D = molecular diffusivity
ν_a = kinematic viscosity of air
ν_w = kinematic viscosity of water
κ = the Von Karmen constant
ρ_a = density of air
ρ_w = density of water
u_* = shear velocity
$z_0 u_*$ = is given as

$$\frac{1}{z_0 u_*} = \frac{1}{z_c} \frac{\lambda_1 u_*}{\nu} e^{-u_*/u_{*t}}$$

and

$$\Gamma(u_*) = \Gamma_0 \frac{u_*}{u_{*c}} \exp\left[\frac{-u_*}{u_{*c}} + 1\right]$$

u_{*c} = critical shear stress
u_{*t} = transition shear stress

$$u_* = (C_D)^{1/2} U_a$$

where

C_D = drag coefficient
U_a = wind speed

The drag coefficient is a non-linear function of wind speed derived from formulation described in O'Connor (1983)

$$\frac{1}{\sqrt{C_D}} = \frac{1}{\kappa}\left[ln\ 1000 \cdot \left(\frac{1}{z_e} + \frac{\lambda_1 \sqrt{C_D} U_A}{\nu} \exp(-\sqrt{C_D U_A / u_{*t}})\right)\right]$$

(5.39)

The quantities λ_1, u_{*t}, Γ_0, u_{*c}, and z_e are dependent on the size of the water body and values for these parameters are given in Table 5.46 from O'Connor,

Table 5-46. Transfer-Wind Correlations [O'Connor (1983)]

	λ_1	u_{*t}	Γ_0	u_{*c}	z_e
Small scale	10	9	10	22	0.25
Intermediate	3	10	6.5	11	0.25
Large scale	3	10	5	11	0.35
	2	9	2.5	6.2	0.15

1983); small scale values are for laboratory studies, intermediate scale values are for small scale field sites and large scales are for large lake or ocean scales.

A Fortran implementation which calculates drag coefficients and reaeration coefficients using O'Connor's method is available for the U.S. EPA Center for Exposure Assessment Modeling in Athens. This program requires as input; the size scale of the water body, wind speed at 10 m, (m/sec), air temperature (°C), and water temperature (°C). Values for the drag coefficient and reaeration coefficient are calculated by the program. The program is available through the CEAM bulletin board. A more detailed description of the equation development may be found in O'Connor (1983).

SUPPLEMENT XV: SELECTION OF SOD RATES

Guidance on the Selection of Sediment Oxygen Demand Rates is given in Table 5.47.

Table 5-47. Measured Values of Sediment Oxygen Demand in Estuaries and Marine Systems [Bowie et al. (1985)]

SOD ($g\ O^2/m^2$ day)	Environment	Experimental Conditions	References
0.10±0.03 (12°C) 0.20±0.05 (20°C) 0.22±0.09 (28°C) 0.37±0.15 (36°C)	A North Carolina estuary	45 day incubation of 0.6 liters sediment in 3.85 liters BOD dilution water, light	NCASI (1981)
2.32±0.16 1.88±0.018	Buzzards Bay near raw sewage outfall Buzzards Bay control	In situ dark respirometers stirred, 1-3 days; temperature unknown	Smith et al. (1973)
0.14-0.68 (5°C) 0.20-0.76 (10°C) 0.30-1.52 (15°C)	Puget Sound sediment cores	Laboratory incubations	Pamatmat et al. (1973)
0.05-0.10	San Diego Trough (deep marine sediments)	In situ respirometry for 5-13 hours, 4°C, light	Smith (1974)
1.25-3.9	Yaquina River Estuary, Oregon	Dark laboratory incubators, stirred, 20°C	Martin & Bella (1971)
0.02-0.49	Eastern tropical Pacific	Shipboard incubations, 15°C, stirred, dark	Pamatmat (1971)
0.9-3.0	Baltic Sea	In situ light respirometer stirred, 10°C	Edberg & Hofsten (1973)
0.4-0.71	Baltic Sea	Laboratory incubations, stirred, dark, 10°C	Edberg & Hofsten (1973)
0-10.7	Delaware Estuary (22 stations)	In situ dark respirometry, 13-14°c	Albert (1983)
0.3-3.0	Fresh and brackish waters, Sweden	In situ respirometry, 0-18°C Laboratory cores, 5-13°C	Edberg & Hofsten (1973)

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6. SIMPLIFIED ILLUSTRATIVE EXAMPLES

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This section presents illustrative examples of estuarine modeling using both simple screening procedures and the water quality model WASP4. The examples are provided primarily to serve as templates to facilitate future estuarine WLA analyses. Sample calculations and model inputs are provided as well as background information on the models being used. The reader is referred to other chapters and other guidance manuals for detailed technical guidance.

Screening procedures are provided to demonstrate estuarine analyses conducted without use of computer models. Screening analyses provided herein are based upon simple analytical equations and the more detailed guidance provided in the EPA Report "Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants - Part 2" (Mills et al, 1985).

WASP4 examples are provided to demonstrate model-based estuarine WLA application. WASP4 is a general multi-dimensional model supported and available through the U.S. EPA Center for Exposure Assessment Modeling, Athens, Georgia (requests require 3 double sided double density diskettes). WASP4, a general-complexity water quality model, can be used to simulate a wide range of water quality processes in different types of estuaries. Depending upon the type of estuary/water quality processes simulated, the representative WASP4 input file will vary greatly.

This chapter presents a range of hypothetical estuarine situations designed to be representative examples of general classes of estuarine WLA analysis. The examples used have been simplified to demonstrate basic uses of the different approaches. This chapter does not provide detailed guidance on model selection, model development, calibration, waste load allocation, or all-inclusive instructions on WASP4 use.

Model input files for each WASP4 example are provided in an Appendix to this manual which is available from the Center for Exposure Assessment Modeling on diskette. These input files can be used as templates in simulation of water quality. The templates allow estuarine modelers to modify an existing input file to meet site-specific modeling needs instead of the more time consuming and difficult task of developing the entire input file from scratch.

The examples provided herein consider eight water quality concerns in three basic types of estuarine characterizations:

One-Dimensional Estuary:

- Analytical equation for non-conservative toxic
- Fraction of freshwater method for conservative toxic
- Modified tidal prism method for non-conservative toxic
- Total Residual Chlorine
- Bacteria
- Simple DO depletion

Vertically Stratified Estuary:

- Nutrient enrichment

- Algal production/DO/sediment interaction

Laterally Variant Estuary:

- Ammonia toxicity
- Toxic chemical in water column and sediments

The chapter is divided into four parts discussing:

1. Screening Procedures
2. Screening Examples
3. WASP4 Modeling
4. WASP4 Examples

6.1. Screening Procedures

Often times, valuable information on estuarine water quality impacts can be gained without application of a sophisticated computer model. Simple screening procedures, which can be applied using only a hand calculator or computer spreadsheet, have been developed to facilitate preliminary assessments of toxic and conventional pollutants in estuaries . While these screening procedures may not be suitable as the sole justification for a waste load allocation, they do serve a valuable purpose for initial problem assessment or when available resources (staff, time, and/or field data) are insufficient to allow for more rigorous modeling analysis.

This section provides example descriptions of three screening procedures used for estimating estuarine water quality impacts: analytical equations for an idealized estuary, the fraction of freshwater method, and the modified tidal prism method. These three example procedures are only applicable to steady state, tidal-average one- dimensional estuary problems. All three procedures provide "far-field" calculations (well distanced from the outfall) in contrast to "near-field" predictions very close to the outfall. Far-field calculations are unaffected by the buoyancy and momentum of the wastewater as it is discharged.

These three screening procedures assume that the wastewater is well mixed both vertically and laterally in the estuarine model segment. The latter two screening procedures are described in much greater detail in the document "Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants - Part 2" (Mills et al, 1985). Screening procedures for vertically- and laterally-variant estuaries are also described in the manual but are too complex for example illustration herein. The reader is referred to that document for a thorough discussion of several estuarine screening procedures including explicit instruction on proper application and limitations of the various techniques.

6.1.1. Analytical Equations

Many estuarine analyses can be easily conducted by making certain simplifying assumptions about the estuary and pollutant behavior. The simplifying assumptions common to all three screening techniques presented herein are that the pollutant concentrations do not vary significantly in the lateral or vertical directions (i.e. a one- dimensional system), and that tidal-averaged, steady state conditions are being represented. By making a few additional simplifying assumptions, pollutant behavior from point sources can be described using relatively simple analytical equations. These assumptions are that cross-sectional area, flow, and first-order reaction rates are constant over the length of estuary of interest; and that discharges are sufficiently distant from the upstream or downstream boundary of the estuary.

Three separate equations are available to predict concentrations at any location in the estuary, depending upon whether location of interest is: 1) at, 2) upstream of, or 3) downstream of the point of discharge. Estuary locations are specified as distance downstream of the outfall. Locations upstream of the outfall are represented by negative distances, locations downstream by positive distances. The predicted pollutant concentration, C, at any point in the estuary, x, for a point source at location x=0 can be estimated from the equations (Thomann and Mueller, 1987):

$$C = C_0 = W/(Qa) \qquad x = 0 \tag{6-1}$$

$$C = C_0 * \exp(j_1 x) \qquad x < 0 \tag{6-2}$$

$$C = C_0 * \exp(j_2 x) \qquad x > 0 \tag{6-3}$$

where:

$$a = (1 + 4KE/U^2)^{1/2}$$

$$j_1 = U/2E \ (1 + a)$$

$$j_2 = U/2E \ (1 - a)$$

C = pollutant concentration (M/L^3)

W = point source pollutant load (M/T)

x = distance downstream of discharge (L)

K = first-order decay rate coefficient (1/T)

U = net non-tidal velocity

= freshwater flow/cross-sectional area (L/T)

E = tidal dispersion coefficient (L^2/T)

The net nontidal velocity can be directly determined from freshwater flow data (e.g. USGS) and cross-sectional area (e.g. NOAA hydrographic charts), leaving the tidal dispersion coefficient and first-order loss rate coefficient as the only "calibration" parameters.

Several methods are available for estimating the tidal dispersion coefficient (e.g. Thomann, 1972), the most common of which is calibration to observed salinity or chloride data. Since chloride and salinity behavior can be assumed conservative (i.e. K=0), Equation 6-2 becomes:

$$C = C_0 * \exp(Ux/E), \quad x < 0 \tag{6-4}$$

which can be restated in the form (Thomann and Mueller, 1987):

$$\ln C/C_0 = (U/E) * x \tag{6-5}$$

Equation 6-5 states that the slope of the logarithms of observed salinity versus distance (U/E) can be used to determine E, given an estimate of net freshwater velocity. Specifically, by fitting a line through a plot of salinity vs. distance on semi-log paper, E can be determined as:

$$E = \frac{U(x_2 - x_1)}{\ln(C_2 - C_1)} \tag{6-6}$$

An application of this method is provided in the Screening Examples portion of this section (Subsection 6.2).

The analytical equations provided in Equations 6-1 to 6-3 can also be applied to multiple discharge situations through the principal of superposition. Simply stated, Equations 6-1 to 6-3 are applied to predict pollutant concentrations for each discharger (independent of all other discharges) throughout the estuary. The pollutant concentration distribution throughout the estuary due to all discharges is determined by summation of the predicted concentrations at any location for each individual discharge. This procedure will also be demonstrated as part of the Screening Examples (Subsection 6.2).

6.1.2. Fraction of Freshwater Method

The fraction of freshwater method allows quick estimation of tidal average, steady-state pollutant concentrations resulting from point source or upstream discharge without consideration of reaction losses or gains. The method estimates estuarine flushing and dilution from freshwater and tidal flow by comparing salinity in the estuary to the salinity of local seawater, (i.e. the fraction of freshwater). This method is useful for systems where the assumption of constant cross-sectional area and flow over distance is grossly violated.

The balance of freshwater to seawater is the basis of this screening procedure. The fraction of freshwater in any specified estuarine segment is calculated by examining the salinity ratio to seawater as follows:

$$f_i = \frac{S_s - S_i}{S_s} \tag{6-7}$$

where

f_i = fraction of freshwater in segment i

S_s = salinity of local seawater (ppt)

S_i = salinity in estuary segment i (ppt)

From a different perspective, this ratio can be viewed to define the degree of dilution of freshwater (and pollutants) by seawater. With this in mind the total dilution of a pollutant input can be calculated by multiplying the seawater dilution by the freshwater dilution. This then provides a simple way to calculate concentrations of conservative pollutants. For a location x, including or <u>downstream</u> of the discharge,

$$C_x = f_x \frac{W}{Q} \tag{6-8}$$

where:

f_x = fraction freshwater at location x

W = waste loading rate (M/T)

Q = freshwater inflow (L^3/T)

The right hand side of Equation 6-8 can be divided into two distinct terms. The term W/Q represents the classical approach to determining dilution in rivers caused by upstream freshwater flow. The second term, f_x, accounts for the further dilution of the river concentration by seawater. Equation 6-8 also predicts concentrations at the point of discharge, C_o, by using the corresponding fraction of freshwater at that location, f_o.

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

$$C_x = f_o \frac{W}{Q} \frac{S_x}{S_o} \tag{6-9}$$

where:

f_o = fraction of freshwater at discharge location

S_x = salinity at location x

S_o = salinity at discharge location

Equations 6-8 and 6-9 can be used to predict conservative pollutant concentrations at all locations upstream and downstream of a discharge. The frac-upstream and downstream of a discharge. The fraction of freshwater method can also be applied to estimate pollutant concentrations in one-dimensional branching estuaries. The calculations become more tedious than those discussed here, but can still be applied in most cases using only a hand calculator. The reader is again referred to Mills et al. (1985) for a thorough discussion of this topic.

6.1.3. Modified Tidal Prism Method

The modified tidal prism method estimates tidal dilution from the total amount of water entering the estuary (or estuarine segment) from tidal inflow, (i.e. the tidal prism). It is more powerful than the fraction of freshwater method because it can consider not only tidal dilution but also non-conservative reaction losses. This method divides an estuary into segments whose volumes (and lengths) are calculated considering low tide volumes and tidal inflow. The tidal prism (or tidal inflow) is compared for each segment to total segment volume to estimate flushing potential in that segment over a tidal cycle. The modified tidal prism method assumes complete mixing of the incoming tidal flow with the water resident in each segment.

The first step in the modified prism method divides the estuary into segments. Each downstream segment volume is equal to the upstream low tide volume plus the tidal inflow over a tidal cycle. This results in increasing segment size as segments are defined seaward. Data on freshwater inflow and tidal flow (or stage) are required for the calculation.

Estuarine segments are defined starting at the fall line and proceeding seaward. An initial segment (referred to as segment 0) is located above the fall line and has a tidal prism volume (P_0) supplied totally by freshwater inflow over one tidal cycle:

$$P_0 = Q\,T \qquad (6\text{-}10)$$

where:

P_0 = tidal prism of segment 0 (L^3)
Q = freshwater inflow (L^3/T)
T = length of tidal cycle (T)

The low tide volume (V_0) in this section is defined as the low tide volume of the segment minus inter-tidal volume, P_0.

Segment volumes starting from segment 1 are defined proceeding seaward such that the low tide volume of segment i (V_i) is defined as the low tide volume of the previous segment plus the inter-tidal volume, expressed as:

$$V_i = V_{i-1} + P_{i-1} \qquad (6\text{-}11)$$

This results in estuarine segments with volumes (and lengths) established to match the local tidal excursion.

Once all segments are defined, an exchange ratio (r_i) can be calculated for each segment as:

$$r_i = \frac{P_i}{P_i + V_i} \qquad (6\text{-}12)$$

This exchange ratio represents the portion of water associated with a segment that is exchanged with adjacent segments during a tidal cycle. This is also equivalent to the inverse of the segment flushing time (in terms of tidal cycles, not actual time) and is important for calculations of reaction losses.

The tidal prism method can be applied in conjunction with the fraction of freshwater method to estimate non-conservative pollutant concentrations in cases where decay and flushing play an approximately equal role in reducing pollutant concentrations. The equations are (Dyer, 1973):

- segment at the outfall,

$$C_d = f_d\,\frac{W}{Q} \qquad (6\text{-}13)$$

- segments downstream of the outfall,

$$C_i = C_d\,\frac{f_i}{f_d}\prod_{i=1}^{n}(B_i) \qquad (6\text{-}14)$$

- segments upstream of the outfall:

$$C_i = C_d\,\frac{S_i}{S_d}\prod_{i=1}^{n}(B_i) \qquad (6\text{-}15)$$

where:

$$B_i = \frac{r_i}{1-(1-r_i)\,e^{-Kt}} \qquad (6\text{-}16)$$

C_i = non-conservative constituent mean concentration in segment "i" (M/L^3)
C_d = conservative constituent mean concentration in segment of discharge (M/L^3)
r_i = the exchange ratio for segment "i" as defined by the modified tidal prism method (dimensionless)
n = number of segments away from the outfall (i.e. $n=1$ for segments adjacent to the outfall; $n=2$ for segments next to these, etc.)
K = first-order decay rate ($1/T$)
t = segment flushing time

= (1/r_l) • Tidal Period (T)

An illustrative example demonstrating application of this technique is provided in the following section of this chapter.

6.2. Screening Examples

The screening procedures described herein can be used to describe a wide range of water quality considerations. This section provides simple illustrative examples designed for three different situations. The examples are simple by design, in order to best illustrate capabilities and use of the procedures. The range documented herein provides a base which can be expanded to consider many water quality concerns.

This section provides a description of screening procedure application to each of the examples, which can be used as templates for future application. The format describing each case study consists of a brief description of the water quality process(es) of concern, followed by a description of all model inputs, and ending with a discussion of model output. Blank calculation tables are provided for the latter two methods to assist in future application of the procedures.

6.2.1. Example 1 - Analytical Solution for Non-conservative Toxic

The first three illustrative examples involve a one-dimensional estuary whose pollutant concentrations are simulated in response to point source discharge(s). This type of estuary characterization simulates changes in concentration longitudinally down the length of the estuary.

Estuary widths are typically small enough that lateral gradients in water quality can be considered insignificant. Further, depths and other estuarine features are such that stratification caused either by salinity or temperature is not important. This characterization is usually relevant in the upper reaches of an estuary (near the fall line) and in tidal tributaries. These screening examples are also designed to represent only steady state, tidally-averaged conditions. Temporal changes in water quality related to changes in pollutant loads or upstream flows, or intra-tidal variations, are not represented. Application of the analytical equations requires the additional assumption that flows, cross-sectional areas, and reaction rates are relatively constant over the length of the estuary.

The first example consists of a wasteload allocation for total residual chlorine (TRC) for a single discharger on a tidal tributary (see Figure 6-1). The goal of the wasteload allocation is to determine the maximum amount of chlorine loading which will just meet the water quality standard of 0.011 mg/l at critical environmental conditions.

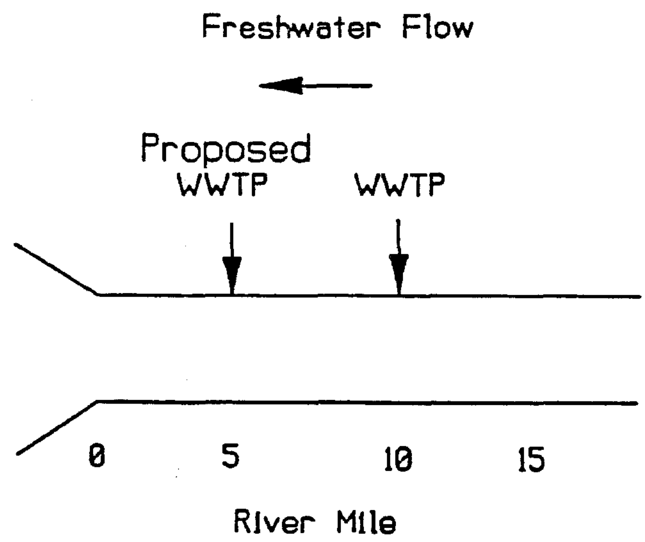

Figure 6-1. Schematic of tidal tributary for analytical equation example.

One survey is available with data on salinity and TRC throughout the estuary. The pertinent information for this estuary/discharge situation is provided in Table 6-1.

The wasteload allocation will proceed by accomplishing three steps:

1. Determine dispersion coefficient

2. Determine decay rate

3. Determine maximum allowable load at critical conditions

Table 6-1. Observed Conditions During Survey

Upstream Flow:	4000 cfs	
Discharge Flow:	300 cfs	
Discharge Conc.:	2 mg/L	
Estuary Cross-Sectional Area:	20,000 ft^2	
Observed Data-		
River Mile	Salinity(%)	TRC(mg/L)
2	19	0.04
4	10	0.06
5	8	0.07
6	6	0.08
9	3	0.15
10	2	0.18
12	1	0.07

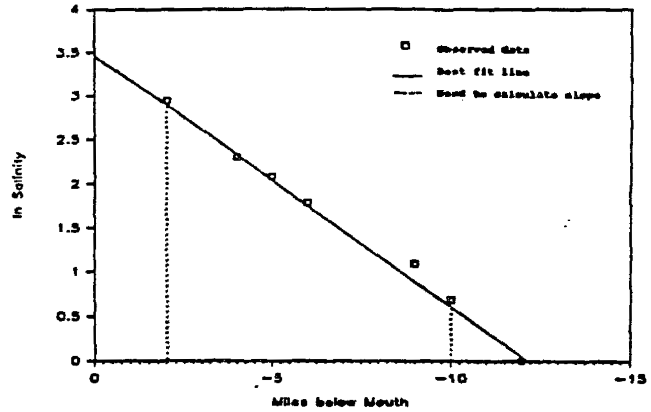

Figure 6-2. Determination of tidal dispersion from salinity data.

The dispersion coefficient is determined by applying Equation 6-6 to the observed salinity data. These data are plotted in Figure 6-2 on semi-log paper as a function of distance from the mouth of the estuary. Note that the analytical equations described herein require that locations upstream of the pollutant source be represented by negative distance units. A straight line is fit through the observed salinity data (Figure 6-2), and two points selected off this line to allow application of Equation 6-6.

For the distances of -10 and -2, the corresponding salinities are 1.8 and 18.1, respectively. The net freshwater velocity is calculated by dividing net freshwater flow (4000 cfs) by cross-sectional area (20,000 ft^2) as 0.20 ft/sec. This velocity is translated into units of miles/day (0.20 ft/sec = 3.28 mi/day), to allow the predicted dispersion coefficient to result in the most commonly used units of mi^2/day. Applying the observed salinity and velocity data to Equation 6-6 results in:

$$E = \frac{3.28\,(-10-(-2))}{\ln\,(1.8/18.1)} \qquad (6\text{-}17)$$

$$= 11.4\, mi^2/day$$

The second step in the wasteload allocation process for this example is calibration of the first-order rate coefficient describing TRC decay. This is accomplished by determining the expected range of values from the scientific literature, and applying different values from within this range to Equations 6-1 to 6-3. The decay rate coefficient which best describes the observed data, and is consistent with the scientific literature, is selected as the calibration value. For this example, acceptable decay rate coefficients were found to range from 0.5 to 5.0/day. Figure 6-3 shows plots of model predictions versus observed data for rate coefficients of 0.5, 1.0, and 5.0/day. The value of 1.0/day best describes the observed data, and is therefore selected as the calibration value. The required calculations for predicting these concentrations throughout the estuary are demonstrated in Table 6-2.

Table 6-2. Predicted Concentrations Throughout Estuary Under Observed Conditions

Inputs			
Q = 4000 cfs	K = 1/day	E = 11.4 mi^2/day	U = 3.28 mi/day
River Mile	Distance Below Discharge (x)	Equation	Predicted Concentration (mg/L)
0	10	6-3	0.004
1	9	6-3	0.005
2	8	6-3	0.007
3	7	6-3	0.010
4	6	6-3	0.013
5	5	6-3	0.017
6	4	6-3	0.023
7	3	6-3	0.031
8	2	6-3	0.041
9	1	6-3	0.055
10	0	6-1	0.073
11	-1	6-2	0.054
12	-2	6-2	0.040
13	-3	6-2	0.029
14	-4	6-2	0.022
15	-5	6-2	0.016

The final step in the wasteload allocation process is to determine the maximum allowable load under critical environmental conditions. Equation 6-1 predicted the concentration at the point of mix as a function of pollutant load; this equation can be rearranged to determine the loading required to obtain a specific concentration under given environmental conditions.

$$W_d = C \bullet Q \bullet a \qquad (6\text{-}18)$$

where:

W_d = allowable pollutant load [M/T]

Q = net freshwater inflow [L^3/T]

C = desired concentration [M/L^3]

a = $(1 + 4KE/U^2)^{1/2}$ [dimensionless]

For wasteload allocation purposes, model parameters should be representative of critical environmental conditions. Some parameters (e.g. upstream flow) will be dictated during specification of critical conditions. Engineering judgement is usually required for many parameters to determine how (if at all) they are expected to change from observed to critical environmental conditions. For this example, the critical

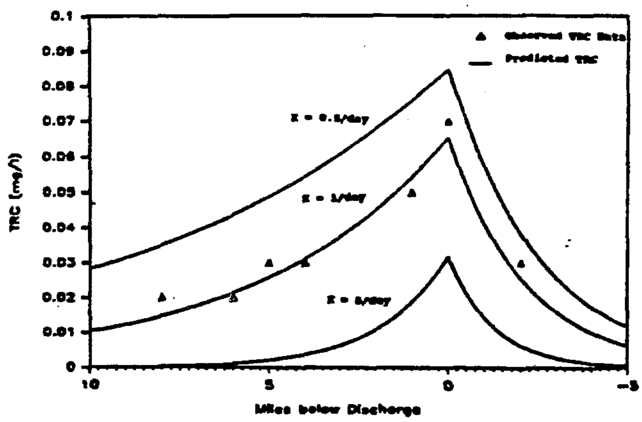

Figure 6-3. Calibration of TRC decay rate.

environmental condition is the drought freshwater flow of 2000 cfs. Since net velocity is directly related to flow (U = Q/A), the velocity under critical conditions is recalculated as 1.64 mi/day. Environmental conditions not expected to change under critical conditions for this example are the tidal dispersion coefficient, pollutant decay rate coefficient, and cross-sectional area. The tidal dispersion coefficient and cross- sectional area are often relatively insensitive to upstream flow in estuarine systems.

The pollutant decay rate may change significantly between observed and critical conditions. Caution should be used in projecting future conditions that the same process(es) that comprised the observed loss rate will be applicable under future projection conditions. For example, a loss rate that includes settling which was calibrated to high freshwater flow conditions may not be directly applicable to future drought flow simulations. The best procedure is to perform sampling surveys during periods as close to critical environmental conditions, to minimize the degree of extrapolation required.

For this example, Equation 6-16 is used to calculate the allowable loading of chlorine to meet the water quality standard as

$$Wd = 0.01\ mg/l * 2000\ cfs * 4.24 * 5.39$$
$$= 457\ pounds/day.$$

Note that 5.39 is a lumped units conversion factor representing (lbs/day)/(cfs*mg/l). Given that the treatment plant flow is assumed to remain constant at 80 cfs, this translates into an allowable effluent concentration of:

$$C_d = 457\ pounds/day\ /\ 80\ cfs\ /\ 5.39 = 1.06\ mg/l$$

To demonstrate a multiple discharge situation, the effect of a proposed second discharge on estuarine TRC concentrations at critical environmental conditions will be evaluated. The specifics of this discharge are:

Location: River mile 5
Flow: 40 cfs
Concentration: 2 mg/l

Table 6-3 demonstrates the steps involved in evaluating multiple discharges. Column (4) is based upon information in Columns (2) and (3) and represents the incremental impact caused by the original discharge.

Table 6-3. Predicted Concentrations Throughout Estuary for Multiple Discharge Situation

	Discharge 1			Discharge 2			Sum
River Mile	Distance Below Discharge (x)	Equation	Concentration	Distance Below Discharge (x)	Equation	Concentration	Total concentration
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
0	10	6-3	0.007	5	6-3	0.007	0.014
1	9	6-3	0.009	4	6-3	0.009	0.018
2	8	6-3	0.011	3	6-3	0.012	0.023
3	7	6-3	0.014	2	6-3	0.015	0.029
4	6	6-3	0.018	1	6-3	0.019	0.037
5	5	6-3	0.022	0	6-1	0.024	0.046
6	4	6-3	0.028	-1	6-2	0.016	0.044
7	3	6-3	0.035	-2	6-2	0.011	0.046
8	2	6-3	0.044	-3	6-2	0.008	0.052
9	1	6-3	0.056	-4	6-2	0.005	0.061
10	0	6-1	0.071	-5	6-2	0.004	0.075
11	-1	6-2	0.049	-6	6-2	0.002	0.051
12	-2	6-2	0.033	-7	6-2	0.002	0.035
13	-3	6-2	0.023	-8	6-2	0.001	0.024
14	-4	6-2	0.016	-9	6-2	0.001	0.017
15	-5	6-2	0.011	-10	6-2	0.001	0.012

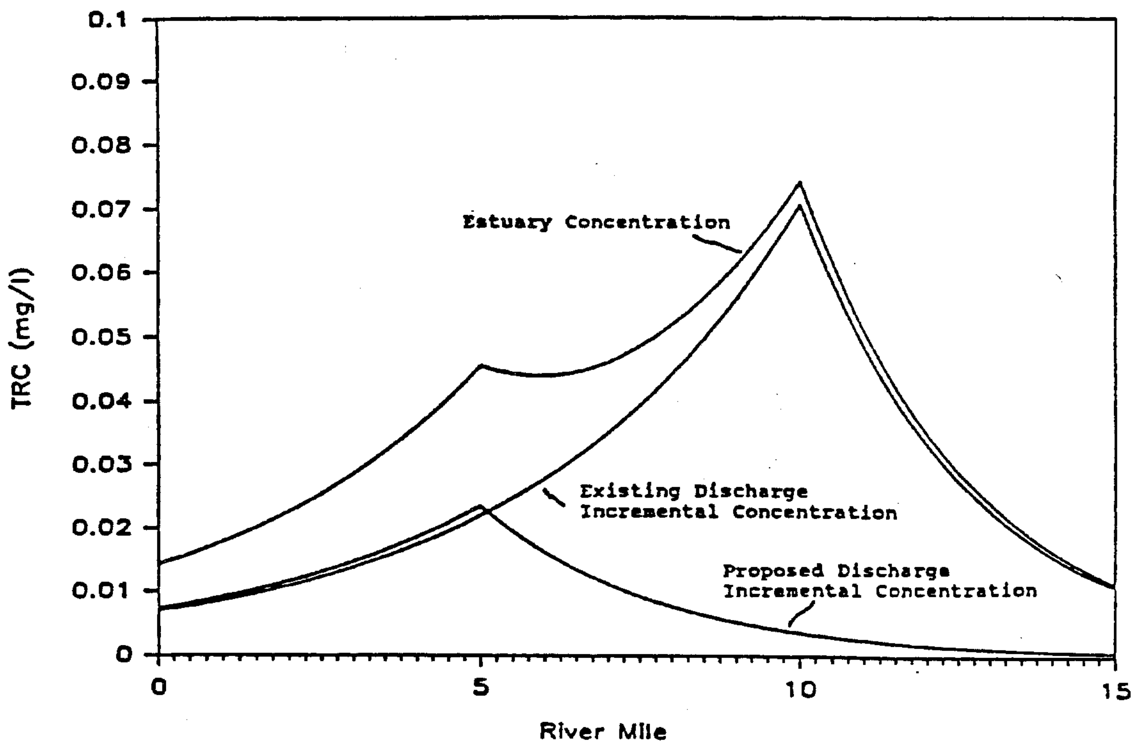

Figure 6-4. Estuary TRC concentration in response to two discharges.

Column (7) is based upon information in Columns (5) and (6) and represents the incremental impact caused by the proposed discharge. Column (8) represents the expected concentration distribution throughout the estuary, and consists of the sum of incremental concentrations from columns (4) and (7). The results of this analysis are shown graphically in Figure 6-4.

6.2.2. Example 2 - Fraction of Freshwater Method for Conservative Toxic

The next two examples also involve one dimensional estuaries, but do not require the assumption of constant flows and cross-sectional areas throughout the estuary. Instead, the estuary is divided into a sequence of segments used to simulate longitudinal water quality differences. For analysis purposes each segment s considered of uniform quality. A single segment describes water quality across the entire width of the estuary, consistent with the assumption of lateral homogeneity. Similarly, a single segment is also used to describe water quality from surface to bottom consistent with the lack of vertical stratification.

The example discussed in this section involves consideration of conservative pollutant behavior, and is amenable to analysis using the fraction of freshwater method. Figure 6-5 shows a schematic of the estuary and how it is compartmentalized into 15 segments.

Table 6-4 serves as a worksheet for calculating conservative pollutant concentrations using this method.

Four inputs are required for the worksheet (Table 6-4):

- Freshwater inflow to the estuary, Q
- Salinity of seawater at the downstream boundary, S_s
- Pollutant loading rate, W_d
- Salinity of each segment, S_i

The location of these inputs are denoted in Table 6-4 by the underscore (__) character. Table 6-5 contains input values obtained for the first example. Freshwater inflow is 2,000 cmd, the salinity of local seawater is 30 ppt, and the loading rate of pollutant is 10,000 g/day. These inputs, in conjunction with Equations 6-7 to 6-9, allow completion of the calculation table.

The first calculation in determining the pollutant distribution is to determine the fraction of freshwater, f_i, for each segment. This is obtained from Equation 6-7, and applied to each model segment. These results are entered into the third column of the worksheet in Table 6-4. The second calculation required is to divide the fraction freshwater in each segment by the fraction of freshwater in the segment receiving discharge. These values are entered into the fourth column of Table 6-4.

Table 6-4. Calculation Table for Conservative Pollutant by Fraction of Freshwater Method [Mills et al.(1985)]

Freshwater Inflow	Local Seawater Salinity	Load
Q= __cmd	S_s = __ppt	W_d = __g/day

Seg #	Salinity, S_i (ppt)	Fraction of Fresh-water, f_i	f_i/f_d	S_i/S_d	Pollutant Con-centra-tion (mg/L)
0	___				
1	___				
2	___				
3	___				
4	___				
5	___				
6	___				
7	___				
8	___				
9	___				
10	___				
11	___				
12	___				
13	___				
14	___				

Table 6-5. Completed Calculation Table for Fraction of Freshwater Method

Freshwater Inflow	Local Seawater Salinity	Load
Q = 2000 cmd	S_s = 30 ppt	W_d = 10,000 g/day

Seg #	Salinity, S_i (ppt)	Fraction of Fresh-water, f_i	f_i/f_d	S_i/S_d	Pollutant Con-centra-tion (mg/L)
0	1	0.97	1.26	0.14	0.54
1	3	0.90	1.17	0.43	1.66
2	5	0.83	1.09	0.71	2.73
3 ← W_d	7	0.77	1.00	1.00	3.85
4	10	0.67	0.87	1.43	3.35
5	12	0.60	0.78	1.71	3.00
6	14	0.53	0.70	2.00	2.65
7	16	0.47	0.61	2.29	2.35
8	18	0.40	0.52	2.57	2.00
9	19	0.37	0.48	2.71	1.85
10	21	0.30	0.39	3.00	1.50
11	23	0.23	0.30	3.29	1.15
12	25	0.17	0.22	3.57	0.85
13	27	0.10	0.13	3.86	0.50
14	29	0.03	0.04	4.14	0.15

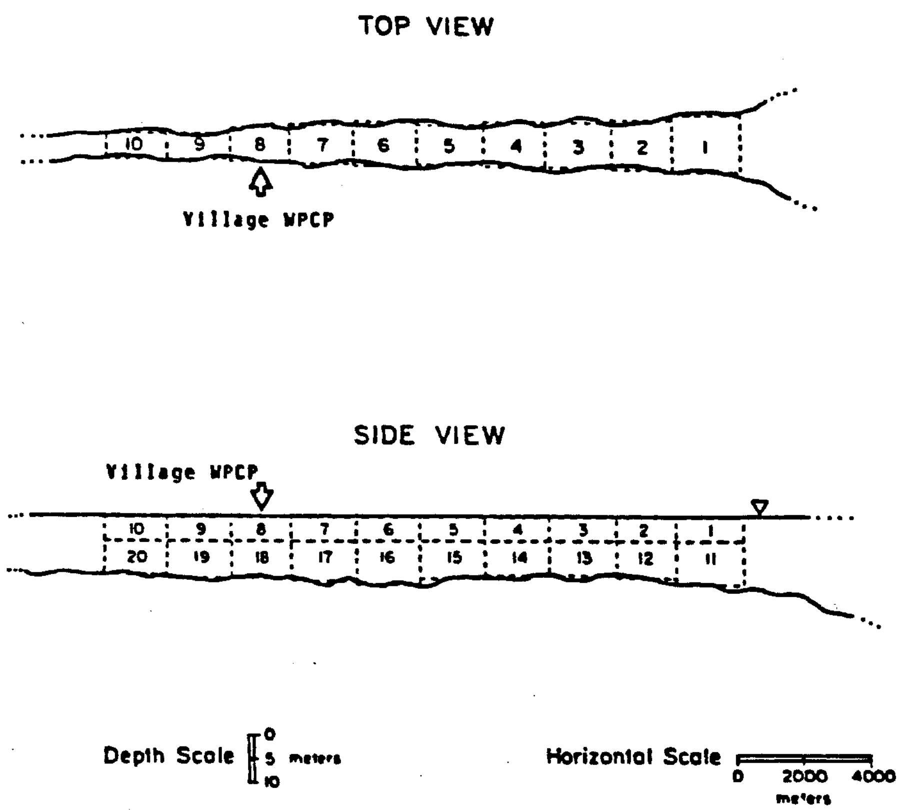

Figure 6-5. Schematic for illustrative vertically stratified estuary.

Table 6-6. Calculation Table for Non-Conservative Pollutant by Modified Tidal Prism Method [Mills et al., (1985)]

Freshwater Inflow	Local Seawater Salinity	Load	Decay	Tidal Cycle
Q = ___cmd	S_s = ___ppt	W_d = ___g/day	K = ___/day	T = ___ days

Seg #	Subtidal Water Volume, V_i 10^6 m^3	Intertidal Water Volume, P_i 10^6 m^3	Salinity, Si ppt	Fraction Fresh, f_i	f_i/f_d	S_i/S_d	Segment Exchange Ratio, r_i	n	$\prod B_i$	Pollutant Concentration mg/L
0	_	_	_							
1	_	_	_							
2	_	_	_							
3	_	_	_							
4	_	_	_							
5	_	_	_							
6	_	_	_							
7	_	_	_							
8	_	_	_							
9	_	_	_							
10	_	_	_							
11	_	_	_							
12	_	_	_							
13	_	_	_							
14										

Seven inputs are required for this worksheet:

- Freshwater inflow to the estuary, Q
- Salinity of seawater at the downstream boundary, S_s
- Pollutant loading rate, W_d
- Salinity of each segment, S_i
- Low tide volume for each segment, P_i
- Inter-tidal volume for each segment, P_i
- First-order decay rate coefficient for each segment, K

The third set of calculations is to divide the salinity in each segment by the salinity in the segment receiving discharge. Finally, pollutant concentrations for each segment are obtained using Equation 6-8 (for segments including and downstream of the one receiving discharge) or Equation 6-9 (for segments upstream of the discharge).

Table 6-5 contains a completed calculation table for the first example, including the expected pollutant distribution. Concentrations are at a maximum of 3.8 mg/l in Segment 12 (the segment receiving discharge), decreasing rapidly in the upstream direction and more gradually proceeding seaward. The assumption of conservative behavior is commonly used in screening level analysis of toxics. The conservative assumption will provide an upper bound of expected pollutant concentrations; if water quality standard violations are indicated for conservative pollutant behavior then application of a fate and transport model may be warranted. Caution should be exercised when considering these results as upper bounds to ensure that the assumption of complete mixing is valid. Incomplete mixing could result in actual concentrations greater than those predicted using this approach.

6.2.3. Example 3 - Modified Tidal Prism Method for Non-Conservative Toxic

This third illustrative example is for the same estuary as described in the previous example (Figure 6-5), but considers non-conservative pollutant behavior. First-order kinetics are used to describe pollutant loss. This situation lends itself to application of the Modified Tidal Prism Method. Table 6-6 serves as a worksheet for calculating non-conservative pollutant concentrations.

The first four inputs are identical to those required for the fraction of freshwater method and are used to calculate the conservative constituent concentration in the segment receiving discharge (Equation 6-13). The fifth and sixth inputs, low tide and inter-tidal water volumes, are used to calculate the exchange ratio for each segment. The final input is the first-order decay rate constant, k. Required model inputs are noted by an underscore (_) in Table 6-6.

Table 6-7. Completed Calculation Table for Non-Conservative Pollutant by Modified Tidal Prism Method

Freshwater Inflow	Local Seawater Salinity	Load	Decay	Tidal Cycle
Q = 2000 cmd	S_s = 30 ppt	W_d = 10,000 g/day	K = 0.01/day	T = 0.48 days

Seg #	Subtidal Water Volume, V_i 10^6 m^3	Intertidal Water Volume, P_i 10^6 m^3	Salinity, Si ppt	Fraction Fresh, f_i	f_i/f_d	S_i/S_d	Segment Exchange Ratio, r_i	n	$\prod B_i$	Pollutant Concentration mg/L
0	5.0	0.5	1	–	–	0.14	0.09	3	0.40	0.22
1	5.5	0.7	3	–	–	0.43	0.11	2	0.62	1.02
2	6.2	1.0	5	–	–	0.71	0.14	1	0.83	2.26
3← W_d	7.2	1.2	7	0.77	1.00	1.00	0.14	–	1.00	3.85
4	8.4	1.4	10	0.67	0.87	–	0.14	1	0.83	2.77
5	9.6	1.8	12	0.60	0.78	–	0.16	2	0.72	2.15
6	11.4	2.0	14	0.53	0.69	–	0.15	3	0.61	1.62
7	13.4	2.4	16	0.47	0.61	–	0.15	4	0.52	1.21
8	15.8	3.3	18	0.40	0.52	–	0.17	5	0.45	0.91
9	19.1	3.6	19	0.37	0.48	–	0.16	6	0.39	0.73
10	22.7	3.8	21	0.30	0.39	–	0.14	7	0.33	0.49
11	26.5	4.2	23	0.23	0.30	–	0.14	8	0.27	0.31
12	30.7	4.4	25	0.17	0.22	–	0.13	9	0.22	0.18
13	35.1	4.6	27	0.10	0.13	–	0.12	10	0.17	0.08
14	39.7	4.8	29	0.03	0.04	–	0.11	11	0.13	0.02

For this example, identical conditions (salinity, freshwater inflow, and loading) are used as the first example, with the primary difference being the addition of a first-order decay rate of 0.5 day^{-1}. The first step in performing the modified tidal prism method is to define the estuarine segmentation using the procedures described previously. That is, segment sizes must be selected such that low tide volume in each segment is equal to the high tide volume for the segment immediately upstream. The required information on tidal prism volumes can be obtained from tidal stage information (tidal gaging stations or NOAA predictions) in conjunction with channel geometry information (from hydrographic maps). Calculation of segment volumes is the most time consuming step of the modified tidal prism method. The information on the sub-tidal and inter-tidal volume of each segment of the example estuary is entered in columns 2 and 3 of Table 6-6. The fraction freshwater is calculated from local salinity values; they are identical to those used for the first example. The segment exchange ratios are calculated from the segment volumes using Equation 6-12. Finally, pollutant concentrations are calculated using: Equation 6-13 for the segment receiving discharge; Equation 6-14 for segments downstream of the discharge; and Equation 6-15 for segments upstream of the discharge.

A completed calculation table is provided for this example in Table 6-7. Pollutant concentrations follow a similar trend as for the first example, but decrease significantly faster in both the upstream and downstream directions. The difference in pollutant concentrations is caused solely by pollutant decay. The greater the distance from the outfall, the greater the difference in predicted concentrations, as longer travel time provides greater opportunity for decay.

A single first-order loss term is used to describe the behavior of many pollutants, even though multiple fate processes may be occurring simultaneously. Rate coefficients for first-order processes are additive, therefore, these multiple processes can be combined into a single "lumped" parameter. Application of this model may include "calibration" of the first-order loss rate to available in-stream pollutant data. As discussed for the analytical equation example, caution should be used in projecting future conditions to insure that the same process(es) that comprised the observed loss rate will be in place under future projection conditions.

6.3. WASP4 MODELING

Deterministic water quality modeling of estuarine systems can often be divided into two separate tasks:

1. Description of hydrodynamics (current, tides, circulation, mixing, etc.).

2. Description of water quality processes.

The WASP4 model was designed to simulate water quality processes, but requires hydrodynamic information as input. This information can be entered into WASP4 by reading the output results from a separate hydrodynamic model of the system or through direct specification of hydrodynamic data in the WASP4 input file. Mixing is simulated through use of dispersion coefficients. Both hydrodynamic and water quality aspects of the WASP model are summarized below. The reader is referred to the WASP4 User's Manual (Ambrose et al., 1988) for a complete description of model theory and use.

6.3.1. WASP Transport

The description of water movement and mixing in estuarine systems using WASP4 always includes advective flows and dispersive mixing. However, the distinction between the real-time description of tidal hydrodynamics compared to the description of tidal-averaged conditions must be made both for flow and dispersion, as values for these processes will differ dramatically depending on the assumption.

In simulating estuaries with WASP4, the modeler must decide between the tidal averaged approach and real time approach. For the tidal averaged approach, hydrodynamic conditions (and water quality) are averaged over a tidal cycle. In the real time approach, calculations are performed on (figuratively) a minute by minute basis simulating intratidal changes.

All of the illustrative modeling examples provided in this manual assume tidally averaged conditions. Under this assumption, tidal flow is characterized as a mixing process, not advective flow. Advective flows represent net freshwater inflow or known advective circulation patterns. In contrast, real time intratidal calculations can also be conducted with WASP4 to simulate tidal variations. Under this condition, variations in freshwater flow, circulation and tidal flow must be specified. For this type of application the use of DYNHYD4, a component of the WASP4 modeling system, is recommended to define the complex hydrodynamics. These are not illustrated explicitly in this manual. All further discussions in this manual focus on tidal averaged conditions.

Turbulent mixing and tidal mixing between water column segments in WASP4 are characterized by dispersion coefficients. These dispersion coefficients, when coupled with a concentration gradient between segments, account for mixing. The dispersion coefficient can be derived from literature estimates but are usually obtained by direct calibration to dye or salinity data.

Structurally the WASP4 program includes six mechanisms for describing transport, all of which are addressed together in one section of the input file. These "transport fields" consist of: advection and dispersion in the water column; advection and dispersion in the pore water; settling, resuspension, and sedimentation of up to three classes of solids; and evaporation or precipitation. Of these processes, advection and dispersion in the water column are usually the dominant processes controlling estuarine water movement and mixing. The other processes, however, also can play a role in pollutant transport depending on specific conditions. These are not elaborated on herein, because they represent complex physio-chemical processes beyond the intent of these simplified examples.

The description of advective flows within WASP4 is fairly simple. Each inflow or circulation pattern requires specification of the routing through relevant water column segments and the time history of the corresponding flow. The flow routing specification is simply the fraction of the advective flow moving from one segment to another. Dispersion requires only specification of cross- sectional areas between model segments, characteristic lengths, and their respective dispersion coefficients. Specific examples of advection and mixing inputs are provided in the illustrative case studies at the end of this chapter.

6.3.2. WASP4 Description of Water Quality

WASP4 is a general purpose water quality model in that it can be used to simulate a wide range of water quality processes. WASP4 contains two separate kinetic submodels, EUTRO4 and TOXI4, each of which serves a distinct purpose. This section briefly describes the capabilities of each kinetic submodel for simulating water quality. It will serve as background information for the illustrative examples, where the specifics of water quality simulation will be provided.

The first kinetic subroutine in WASP4 is EUTRO4. EUTRO4 is a simplified version of the Potomac Eutrophication Model, PEM (Thomann and Fitzpatrick 1982), and is designed to simulate most conventional pollutant problems (i.e. DO, eutrophication). EUTRO4 can simulate concentrations of up to eight state variables (termed systems by WASP4) in the water column and sediment bed. These systems correspond to:

System Number	EUTRO4 State Variable
1	Ammonia nitrogen
2	Nitrate nitrogen
3	Inorganic phosphorus
4	Phytoplankton carbon
5	Carbonaceous BOD
6	Dissolved oxygen
7	Organic nitrogen
8	Organic phosphorus

EUTRO4 can be used to simulate any or all of these parameters and the interactions between them. The WASP4 users manual discusses in detail all of the possible interaction between state variables.

Three of the illustrative examples provided at the end of this chapter will focus upon the more common applications of EUTRO4: simple DO, algal nutrients, and eutrophication. The first EUTRO4 example considers a simple model simulating CBOD, ammonia nitrogen (NH_3-N), and DO. This type of model complexity is most often used when algal impacts are considered unimportant. This corresponds to the "modified Streeter-Phelps" model described in the WASP4 users manual. The second EUTRO4 example considers algal nutrients and simulates total nitrogen and phosphorus concentrations only. This type of simulation is often used when eutrophication is of concern, but resources or data are insufficient to allow application of a complex eutrophication model. The final EUTRO4 example simulates all aspects of the eutrophication process, and includes all eight state variables simulated by WASP4.

The TOXI4 submodel is a general purpose kinetics subroutine for the simulation of organic chemicals and metals. Unlike EUTRO4, TOXI4 does not have a specific set of state variables. Instead, TOXI4 simulates up to three different chemicals and three different types of particulate matter of the users choosing. TOXI4 identifies these state variables in terms of WASP4 systems as:

System Number	TOXI4 State Variable
1	Chemical 1
2	Solids type 1
3	Solids type 2
4	Solids type 3
5	Chemical 2
6	Chemical 3

The chemicals can be related (e.g., parent compound-daughter product) or totally independent (e.g., chemical and dye tracer). Reactions specific to a chemical or between chemicals and/or solids are totally at the control of the user, using the flexible kinetic parameters made available by the model. TOXI4 can provide simulation of ionization, sorption, hydrolysis, photolysis, oxidation, bacterial degradation, as well as extra reactions specified by the user. TOXI4 simulates concentrations both in the water column and bottom sediments.

This chapter will provide three illustrative examples using TOXI4: bacterial degradation and dye tracer; ammonia toxicity; and toxic pollutant in water column and sediments. These simulations will provide a broad spectrum of potential TOXI4 applications and demonstrate the use of ionization, equilibrium sorption, volatilization, biodegradation, and general first-order decay.

6.4. WASP4 Examples

The remaining six examples demonstrate the use of WASP4 for estuarine WLA modeling. The purpose of these examples is to provide a set of templates to facilitate future WASP4 modeling for a wide range of estuarine situations. The most useful portion of these examples (for potential WASP4 users) is the line by line description of the WASP4 input files and diskette copies of the files themselves. These descriptions are too detailed for inclusion in the body of the text; they are instead supplied in an Appendix to this manual which is available on diskette from the U.S.E.P.A. Center for Exposure Assessment Modeling. This portion of the chapter will provide background information on each example, describe the types of inputs required, show selected WASP4 model results, and briefly describe WLA issues.

6.4.1. Example 1- Bacteria in a One-Dimensional Estuary

The first illustrative example using WASP4 involves a simple non-branching estuary. The analysis is designed to provide an example which is reasonably realistic. Although not a wasteload allocation in the traditional sense, this example illustrates the use of a modeling study in an analysis of bacterial loads. Since the example is intended only for illustration of the application and potential use of a model, such as WASP4, emphasis is not placed on providing details on data requirements and calibration-validation procedures.

6.4.1.1. Problem Setting

In this example, a single discharger has been identified to the Trinity estuary. The estuary has popular sport and commercial fisheries, including shellfish. A dye study was conducted during March of 1980 and used to identify a 2 km buffer zone within which shellfishing was closed. The buffer zone was identified by computing a one day travel time from the sewage outfall of the city of Harris. The criteria on which the closing of the shellfishery within the buffer zone was based is not dependent upon the bacterial wasteload concentrations, but rather the presence of a discharger. This is often the practice for bacterial loadings. Therefore, the purpose of this study is not to determine whether a reduction in load is necessary but whether the buffer zone is adequately protective of human health and

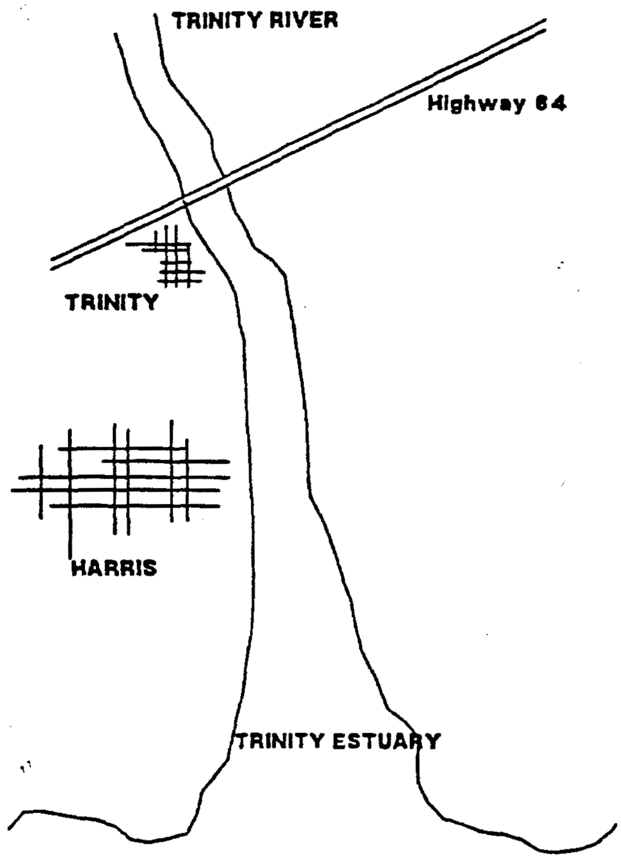

Figure 6-6. The Trinity Estuary.

whether continuing high coliform counts may be attributed to the discharger.

High coliform counts have been detected in the Trinity estuary outside of the buffer zone, leading to periodic closing of the estuary. The area has a large waterfowl population. However, comparisons of fecal coliform and fecal streptococci counts suggests that the problem is of human origin. The pertinent water quality criterion pertains to shellfishing and the applicable standard is 70 counts/100 ml. The criterion for fishing is 1000 counts/100 ml. A summary of the problem setting and treatment plant data is presented in Figure 6-6 and Table 6-8.

6.4.1.2. System Characteristics

The Trinity estuary is approximately 30 km long and receives flow from the Trinity river. The estuary is relatively regular in shape and has no other major tributaries. The city of Trinity is located at the upestuary extremity and the city of Harris is located approximately midway along the estuary. The upstream section of the Trinity river above the fall line is gauged by the USGS. The gauge is located near the crossing of Highway 64. The average monthly flows and temperatures taken at the USGS gauge are provided

Table 6-8. Treatment Plant Effluent Characteristics

Harris City WTP

		· Present
Flow	MGD	17
BOD_5	mg/l	65
$CBOD_u$ (1)	mg/l	130
Total Coliforms	counts/100 ml	1E + 7
DO	mg/l	5

(1) Based on long term BOD estimates of $CBOD_u/CBOD_5$ = 2.0

in Figures 6-7 and 6-8. An analysis of the morphometry of the system indicated that the mean tidal widths and depths could be adequately represented by

$$W = 300\, e^{\,0.0625X} \tag{6-19}$$

and

$$D = 2.43\, e^{\,0.033X} \tag{6-20}$$

where W is the width and D the depth of the estuary, in meters, and X is the distance from the village of Trinity, in kilometers (see Figure 6-6). The village of Trinity does not discharge wastes to the estuary. A water surface elevation gauge is located near the mouth of the estuary, and an analysis of the tidal components was conducted, with the results provided in Table 6-9 and Figure 6-9a. The water surface elevation for the period of interest was then computed from

$$Y = \sum_{i=1}^{7} h_i \cos\left[2\pi t/T_i - P_i\right] \tag{6-21}$$

where Y is the water surface elevation deviation (m) at time t (hrs), h_i is the amplitude (m), T_i the period (hrs), and P_i the phase (in radians) of the seven principal

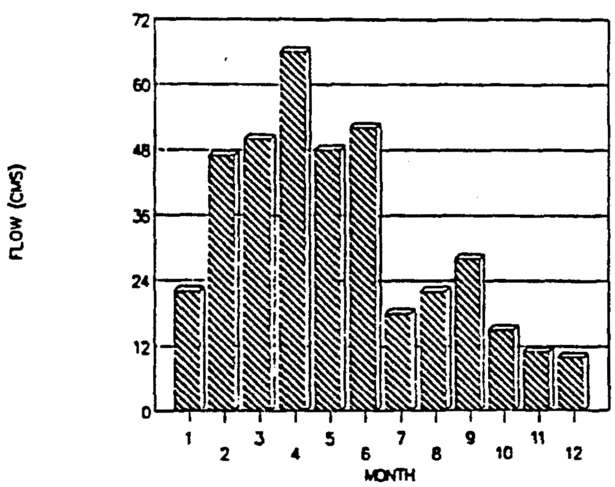

Figure 6-7. Average monthly river flow at the Highway 64 USGS gauge.

Table 6-9. Tidal Periods, Amplitudes and Phases for the Trinity Estuary during March, 1989

Symbol	Name	Period (hours)	Phase (degrees)	Amplitude (cm)
	Semi-Diurnal Components			
M_2	Principal Lunar	12.42	330	23.0
S_2	Principal Solar	12.00	334	5.2
N_2	Larger Lunar Elliptic	12.66	303	4.9
K_2	Luni-solar semi-diurnal	11.97	328	1.6
	Diurnal Components			
K_1	Luni-solar diurnal	23.93	106	15.8
O_1	Principal lunar diurnal	25.82	89	9.8
P_1	Principal solar diurnal	24.07	104	4.9

semidiurnal and diurnal tidal components (see Table 6-9).

6.4.1.3. Supporting Studies

Historical data within the study area are limited. Data are available for temperature at the USGS gauge. Data were available for salinity within the system which was used in model calibration. For this level of study it was determined that no supporting field studies would be conducted.

6.4.1.4. Model Application

For this analysis, model application consisted of: first determining the model network (including morphometry of model segments), then determining appropriate flows and exchange coefficients, and finally simulating bacterial concentrations. The flows for this application were estimated using a one-dimensional hydrodynamic model which was supplied flow data at the riverine boundary and water surface elevations at the mouth of the estuary. A one-dimensional hydrodynamic model, DYNHYD5, is part of the WASP4 modeling system. The WASP4 model may also be coupled with other available hydrodynamic models. The hydrodynamic model was first calibrated and then used to supply flow and volume information to the WASP4 model. Flows were computed over a period of one month in order to examine the effects of successive neap and spring tides. The WASP4 model was then applied to estimate bacterial concentrations.

Several types of information were required to apply WASP. These are described in the Appendix available on disk from the U.S.EPA Center for Exposure Assessment Modeling. The determination of these types of data and their use in this illustrative example is described below.

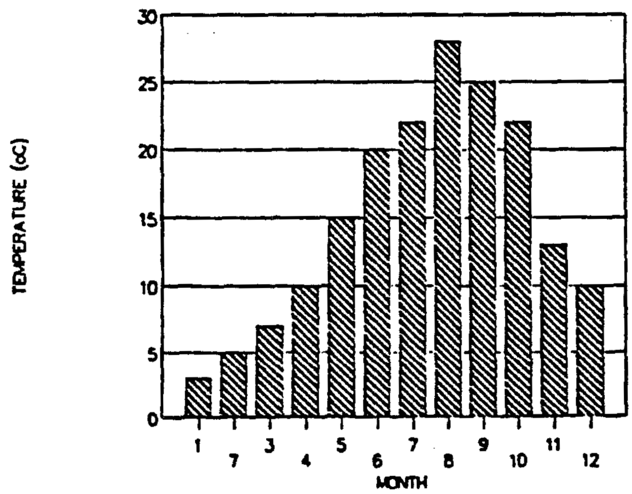

Figure 6-8. Mean monthly temperatures at the Highway 64 USGS gauge.

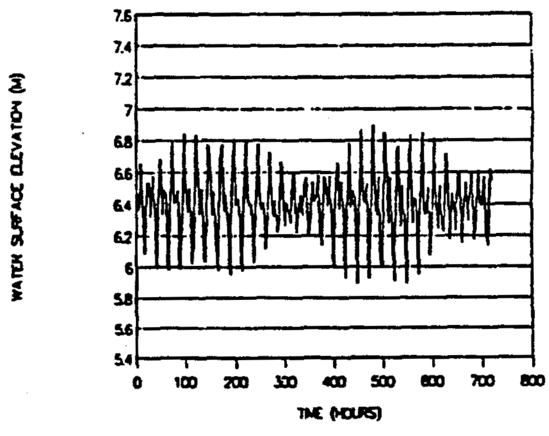

Figure 6-9a. Variations in water surface elevations at the mouth of the Trinity Estuary during March, 1989.

- General model information: The TOXI4 submodel was selected for these simulations. TOXI4 was selected rather than EUTRO4 as a result of its convenience in simulating conservative materials. However, the basic structure and information required in the data input are the same. Five systems were simulated, where system 1 was the bacteria, system 2 was salinity, 3 and 4 were solids (not pertinent to this analysis), and 5 was the dye tracer, treated as a conservative material. This combination of systems is not unique; other combinations could have worked equally as well. The general model information required included the number of model segments, computational time step, length of simulation, and variables (systems) to be modeled.

- Network: The model network refers to how the system is subdivided for analysis. For this application an analysis of the historical data indicated significant longitudinal gradients, with small lateral and vertical variations, allowing application of a one-dimensional model. A network consisting of 15 segments was established. The variations in bottom morphometry and water quality were reasonably regular, and for simplicity segments were delineated every two kilometers. The depths of the segments were determined as well as segment volumes and interfacial areas from available morphometry data. An analysis of the system's morphometry indicated that variations in width and depth were reasonably described by Equations 6-19 and 6-20. The resulting network is illustrated in Figure 6-9b.

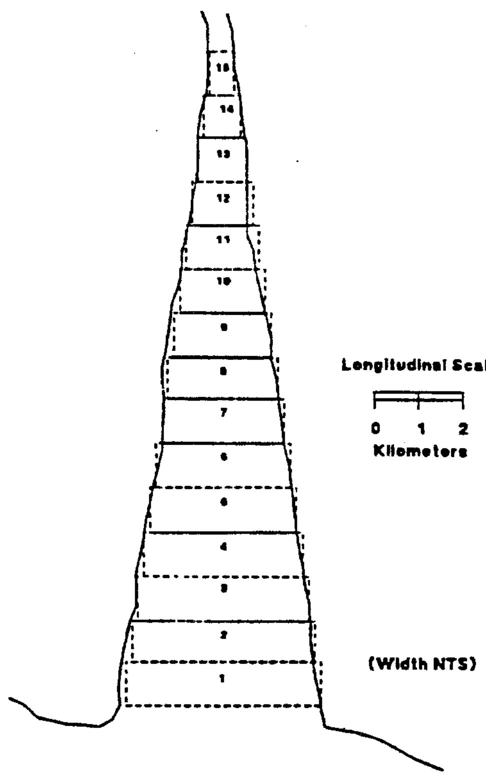

Figure 6-9b. Model network for the Trinity Estuary.

- Dispersion coefficients: Since a hydrodynamic model was used to estimate the effects of tidal mixing, no dispersion was specified. However, where other structures or nonuniformities cause additional dispersion, it may be necessary to specify dispersion rates in other applications. Initial estimates can be derived from the literature and refined through calibration to dye or salinity data.

- Segment volumes: The initial volume of each segment is required, as well as a description of how the volume changes with flow. Volumes are determined from segment width and depth (taken from hydrographic maps) and segment length (user specified). For this application, the segment widths and depths were determined from Equations 6-19 and 6-20, obtained through analysis of the system. Changes in volume in this example were computed by the hydrodynamic model and supplied to the water quality model. Predicted variations in volumes are illustrated in Figure 6-10.

- Flows: Advective flow patterns must be described for segment interfaces, and inflows where they occur. Freshwater inflow data are often available from USGS gaging stations. Tidal data are often available from NOAA. For this application internal flows were estimated using a one-dimensional hydrodynamic model. The internal flows are computed by the hydrodynamic model given the model network and morphometry, the boundary conditions, and factors affecting water movement, such as the bottom roughness. For this application a constant flow of 50 cms was assumed for the Trinity river and a time-varying water surface elevation specified at the ocean boundary (see Figure 6-9b).

- Boundary concentrations: The concentration of bacteria, dye, and salinity must be specified at each system boundary (segments 1 and 15). This information is typically collected during the same water quality surveys used to collect calibration and validation data. For this application it was assumed that the bacterial and dye

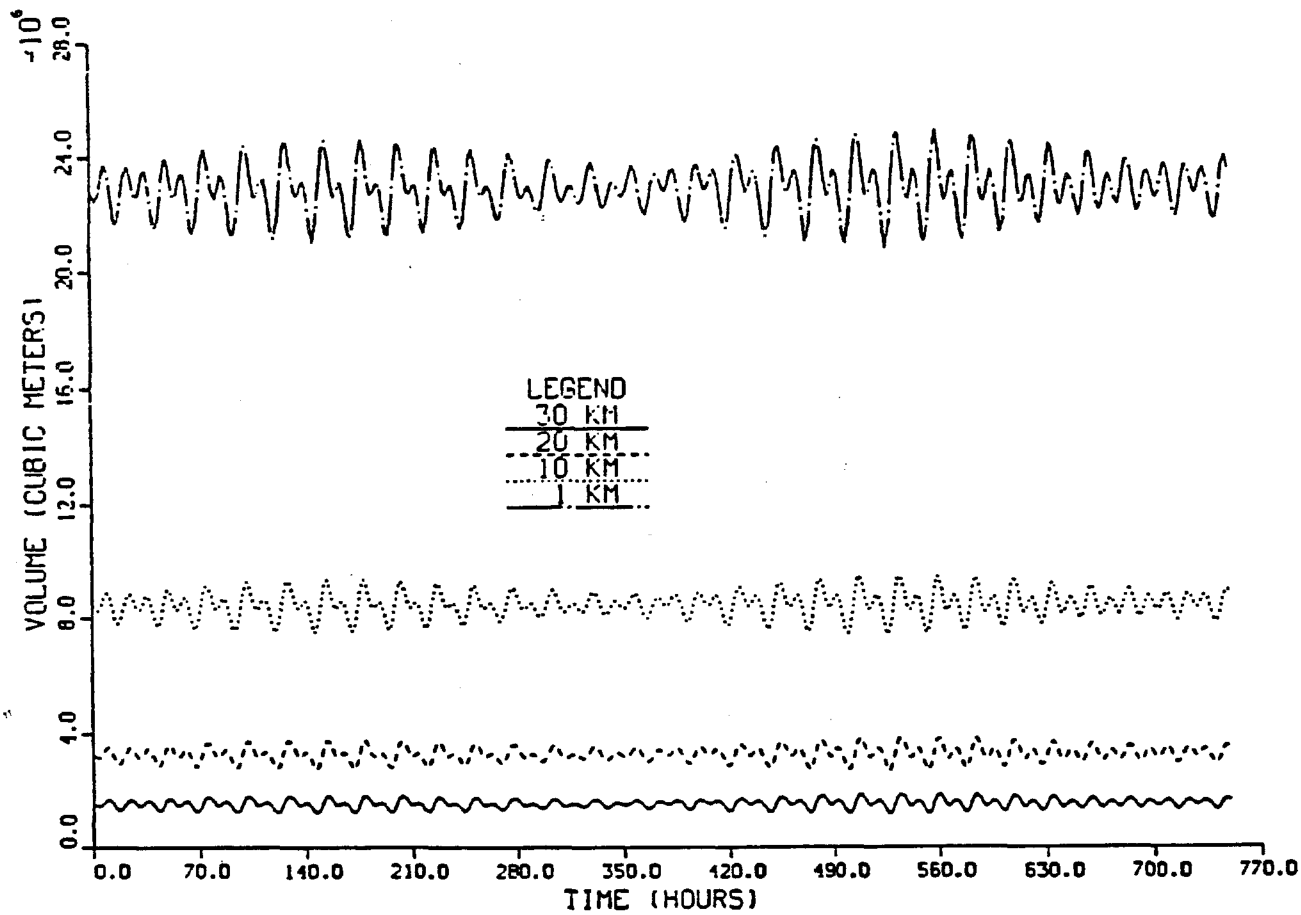

Figure 6-10. Predicted variations in volumes near the mouth, near the midpoint, and at the upper extremity of the Trinity Estuary.

boundary conditions were zero. The salinity at the ocean boundary was specified as 32 ppt.

- Pollutant loads: Pollutant loading rates are required for bacteria and dye for each point source. Loadings can be measured during water quality surveys or taken from discharge monitoring reports. The bacterial loads for this study were computed assuming no chlorination or other disinfection, resulting in the high effluent concentrations given in Table 6-8. The loadings were then computed from the discharge rate and bacterial concentration. The equivalent load for organisms was determined by multiplying the effluent concentration (counts/100 ml) by the flow rate which, after unit conversions, yielded counts per day which was then converted to kilocounts per day for input. To convert this back to counts/100 ml, from the output of TOXI4 in units of μg/l, the values were multiplied by 10^{-7} (1 μg (μ count here) = 10^{-6} g (counts), and 100 ml = 0.1 liter).

- Model constants: A first-order rate coefficient is required to describe bacterial decay. Initial estimates can be derived from the literature and refined through calibration to observed bacteria data. For this study, simulations were conducted with no die-off and then with rates of 1.0 day^{-1}. Guidance on selection of bacterial die-off rates is provided in Section 5. Salinity and the dye tracer were treated as conservative materials (no decay was specified).

- Initial concentrations: Concentrations of dye and bacteria in each model segment are required for the beginning of the simulation. For these simulations, since initial conditions were not available, bacterial and salinity simulations were conducted over a 30 day period. The concentrations at the end of that period were then used for the initial conditions in subsequent simulations. The initial conditions of the dye tracer were assumed to be zero, neglecting any background concentrations.

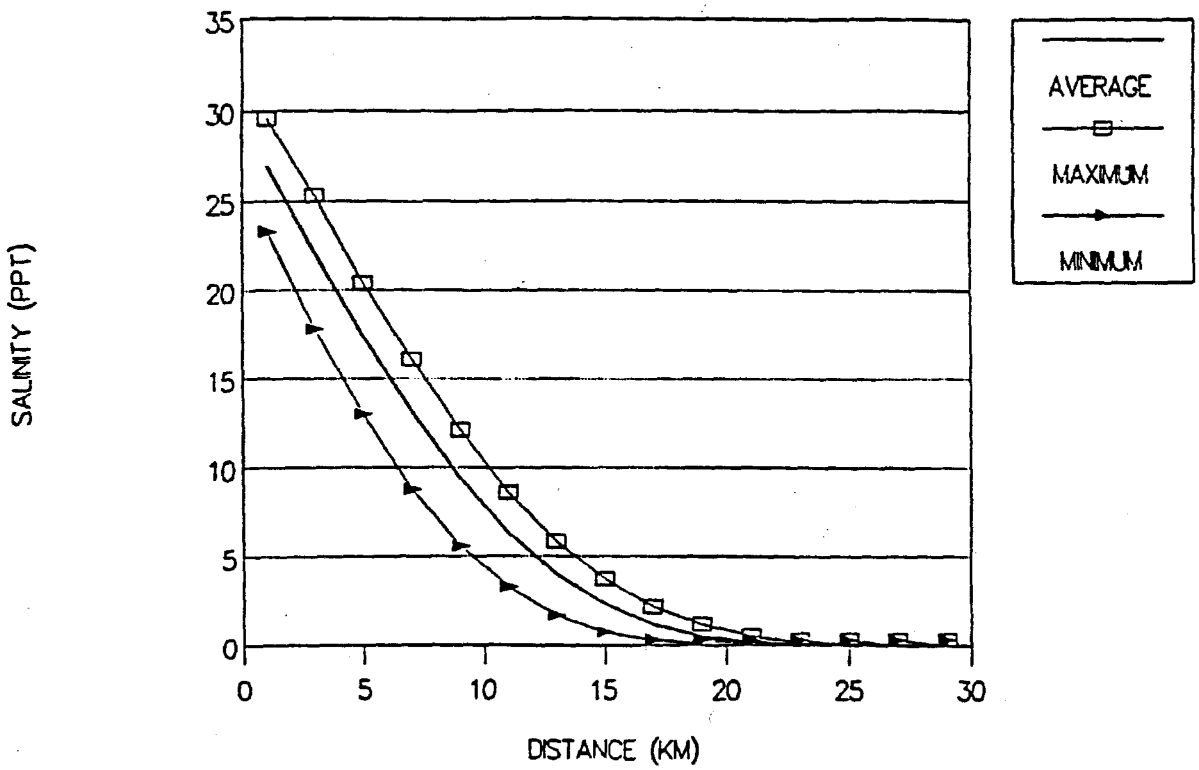

Figure 6-11. Monthly averaged salinities in the Trinity Estuary versus distance upstream from its mouth.

6.4.1.5. Model Simulations

Simulations were first conducted for salinity to insure that model predictions adequately corresponded with field observations. Simulations were conducted over a period of one month. A comparison of the monthly averaged salinities in the Trinity estuary, along with maximum and minimum values, is provided in Figure 6-11. Figures 6-12 and 6-13 illustrate variations of salinity with time at two locations in the estuary: near mouth (Figure 6-12) and near the midpoint of the estuary (15 km up estuary; Figure 6-13).

Following evaluation of simulations of salinity, simulations of dye injections were conducted. In this illustrative example, it was assumed that data were not readily available and no attempt was made to compare simulations with results of the dye study used as the basis for establishing the buffer zone. This comparison would be highly desirable in a practical application. Dye simulations were conducted simulating the release of

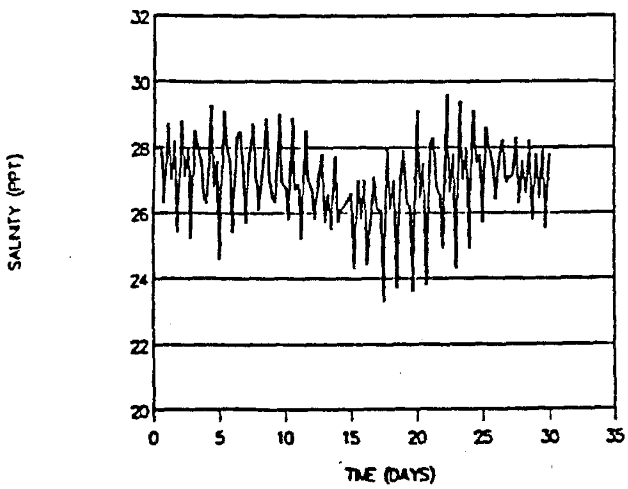

Figure 6-12. Predicted variations in salinity during March, 1989, near the mouth of the Trinity Estuary.

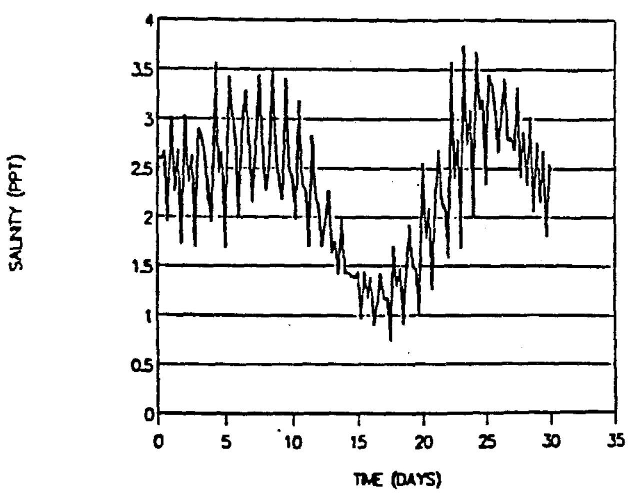

Figure 6-13. Predicted variations in salinity during March, 1989, near the mid-point of the Trinity Estuary.

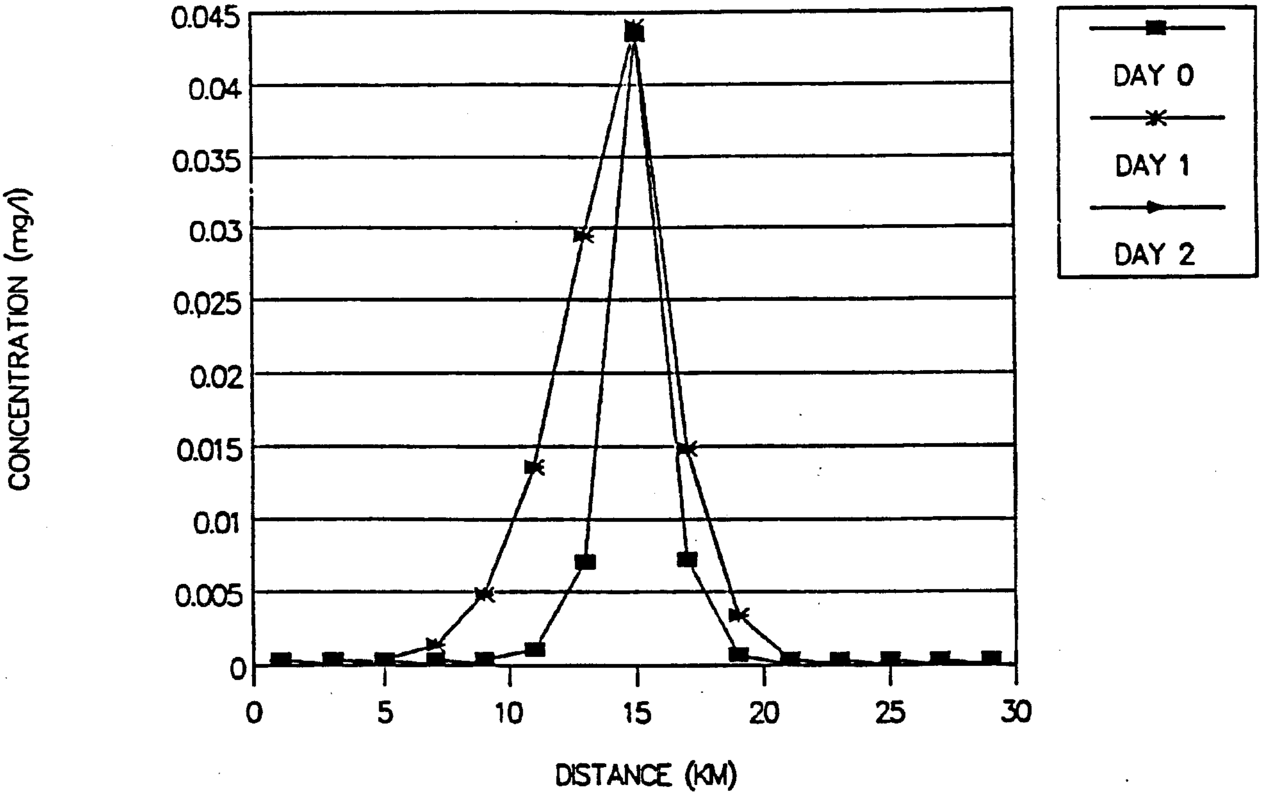

Figure 6-14. Neap tide dye simulations for the Trinity Estuary.

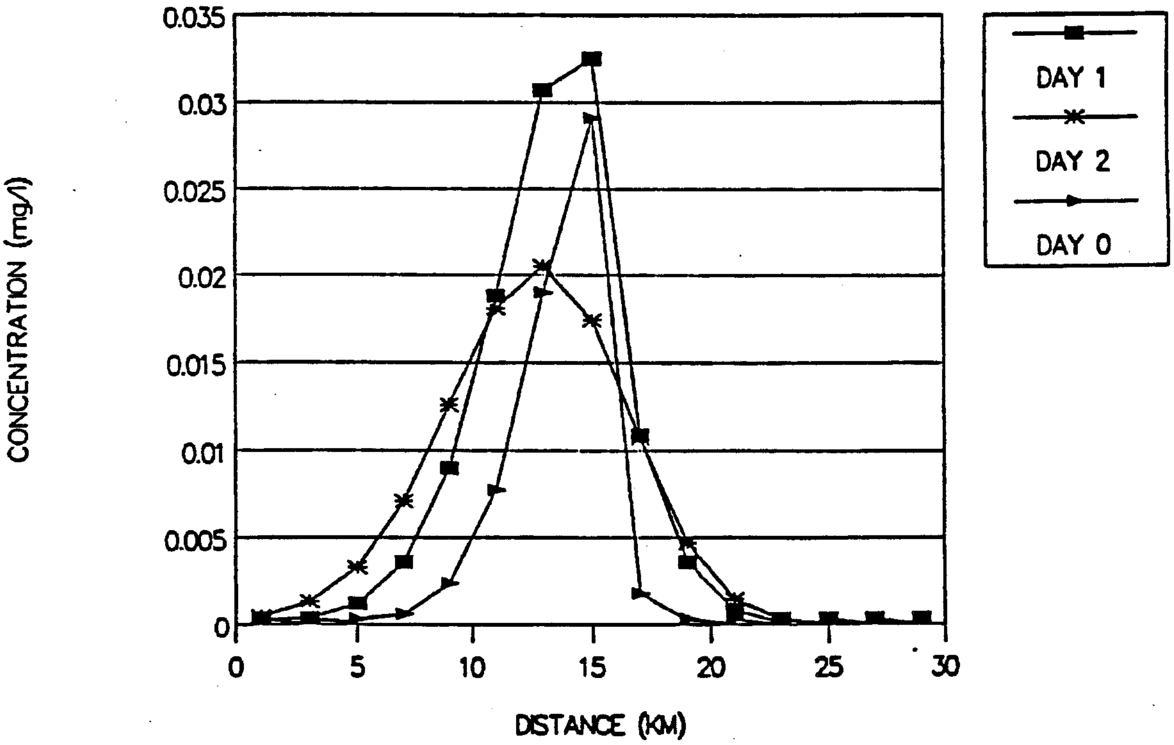

Figure 6-15. Spring tide dye simulations for the Trinity Estuary.

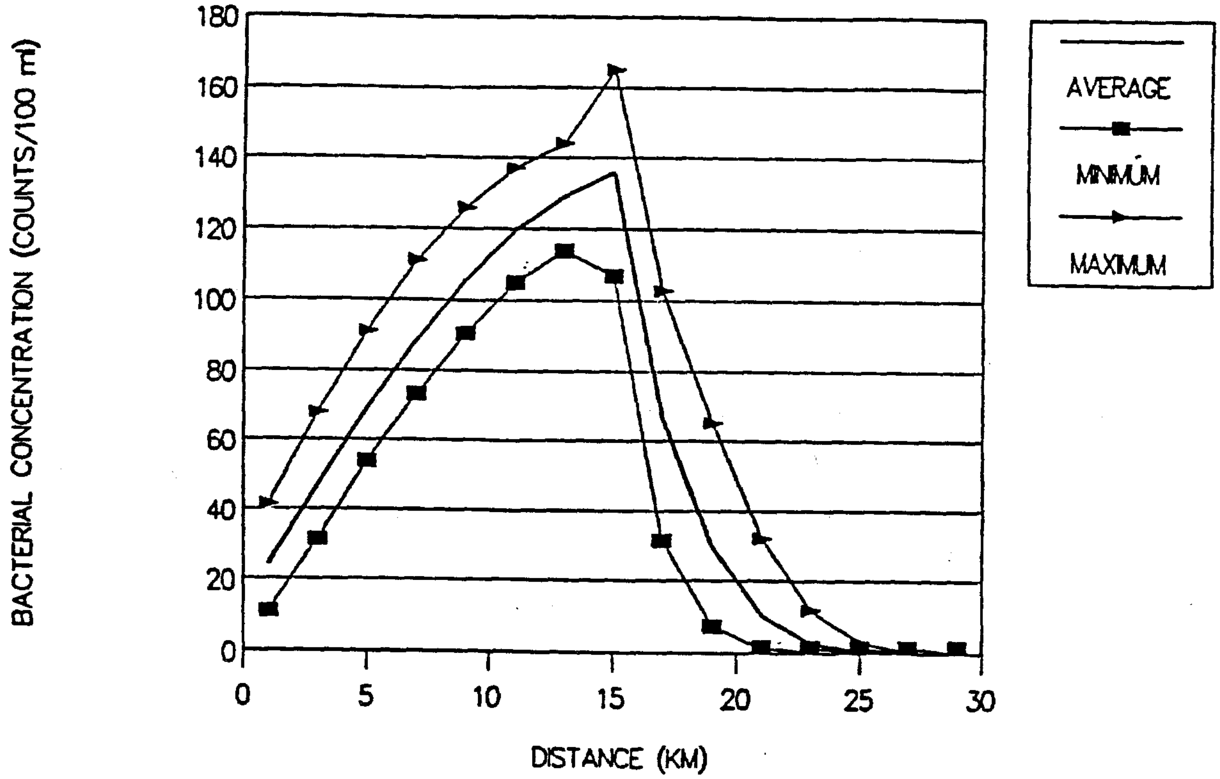

Figure 6-16. Predicted average, minimum and maximum bacterial concentrations for March versus distance from the mouth of the Trinity Estuary assuming no die-off.

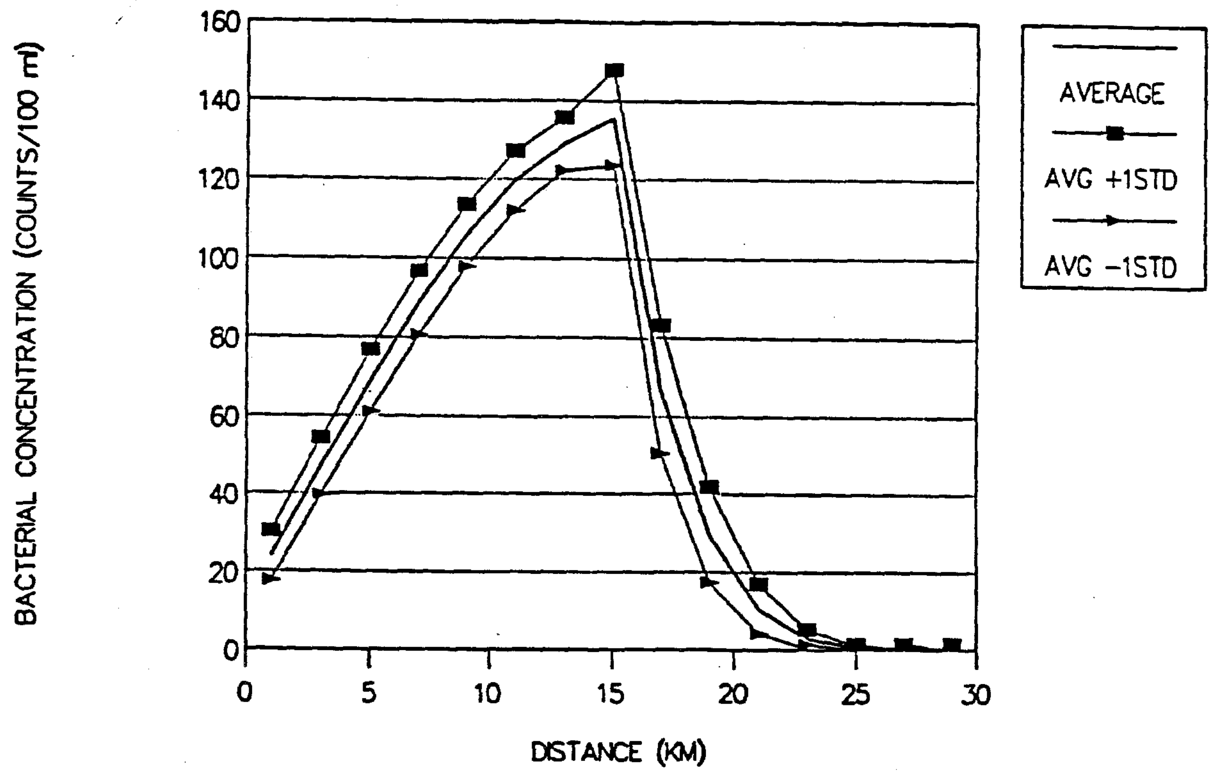

Figure 6-17. Predicted average bacterial concentrations during March, with standard deviations, versus distance from the mouth of the Trinity Estuary assuming no die-off.

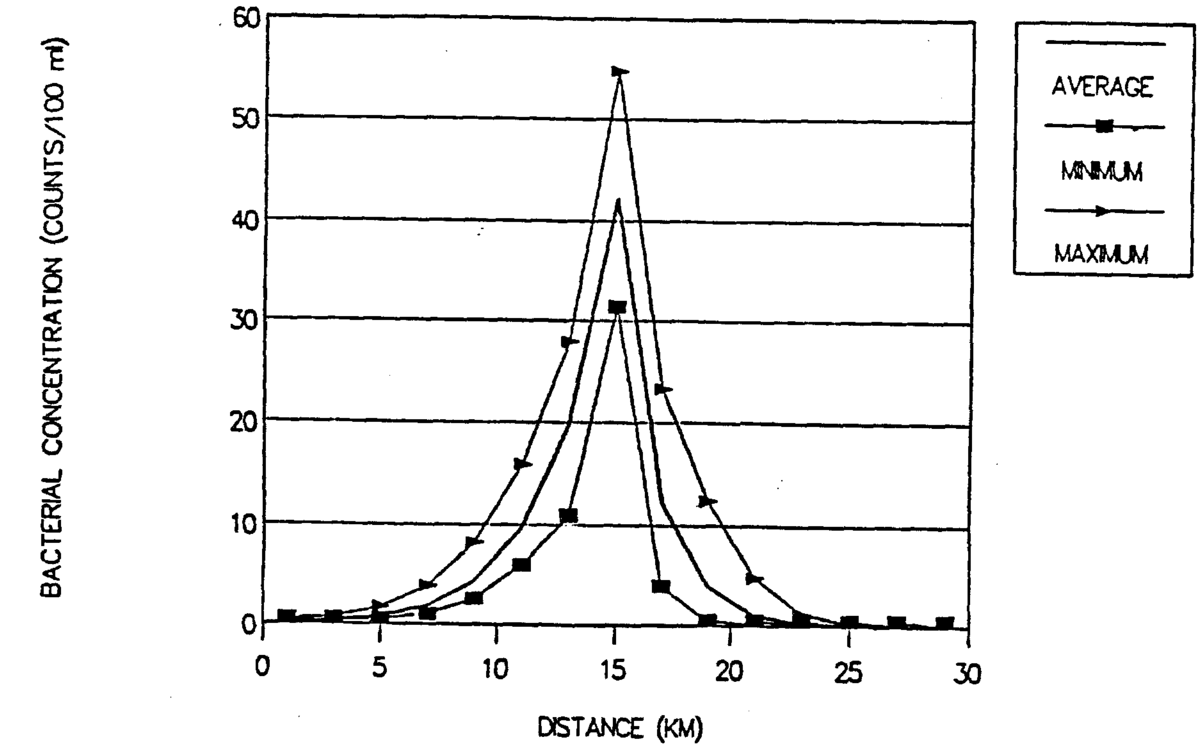

Figure 6-18. Predicted average, maximum and minimum bacterial concentrations during March versus distance from the mouth of the Trinity Estuary assuming a bacterial die-off rate of 1.0 day^{-1}.

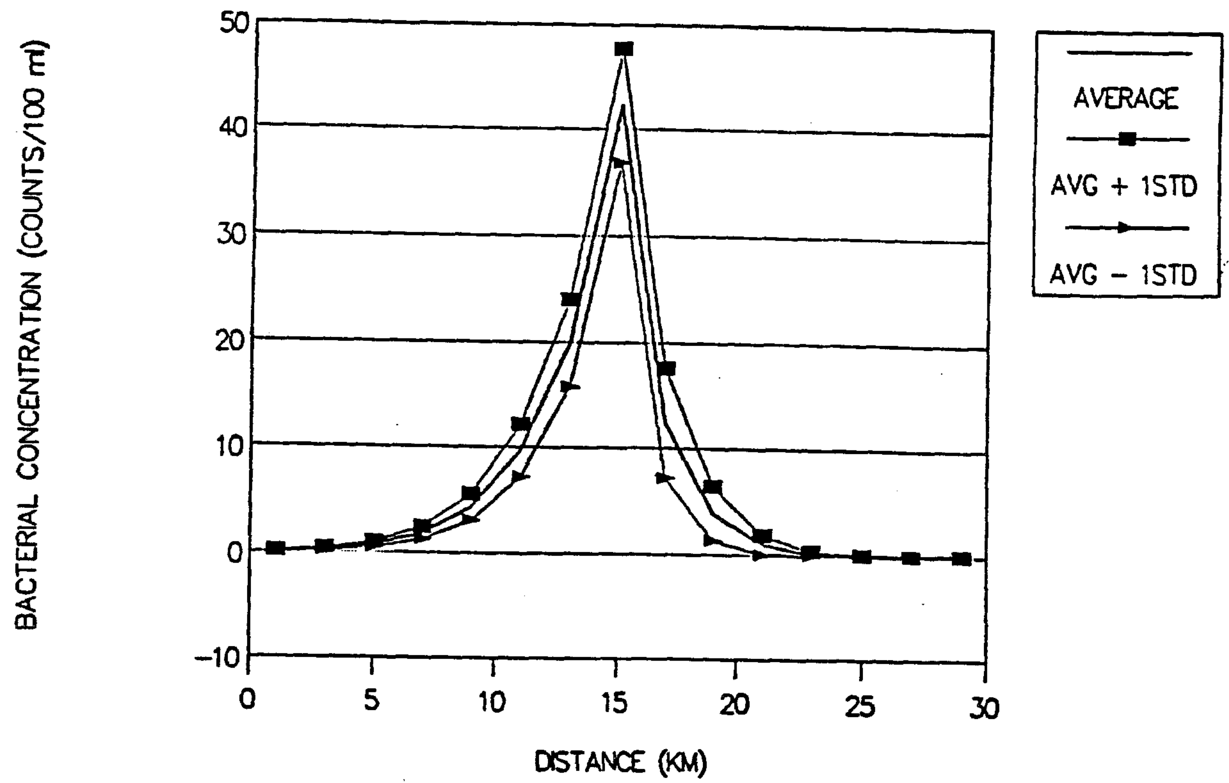

Figure 6-19. Predicted average bacterial concentrations, with their standard deviations, for March versus distance from the mouth of the Trinity Estuary, assuming a bacterial die-off rate of 1.0 day^{-1}.

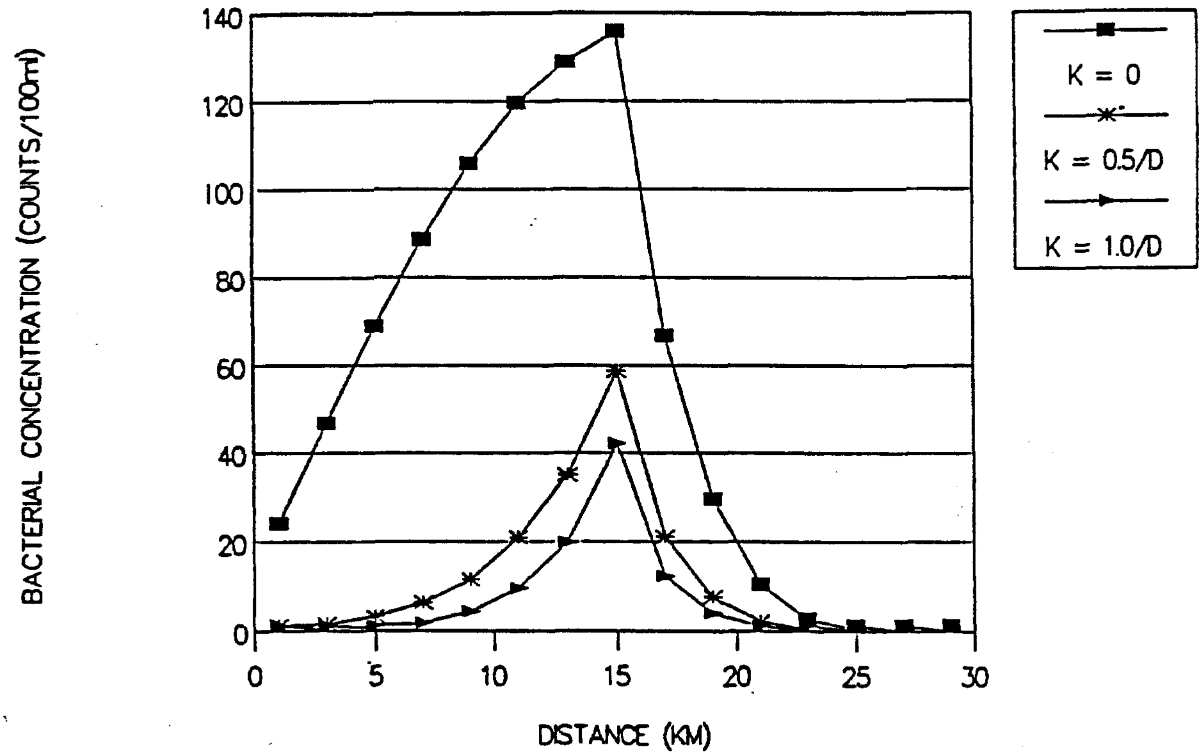

Figure 6-20. Comparison of predicted bacterial concentrations for different die-off rates versus distance from the mouth of the Trinity Estuary.

a slug of dye from the Harris WTP discharge. Simulations included a dye injection near the spring tide and again near the neap tide. The results of these simulations are compared in Figures 6-14 and 6-15. The neap tide simulations indicated little movement of the dye centroid (Figure 6-14), while greater movement occurs during the spring tide (Figure 6-15). However, the centroid of the dye slug was predicted to move less than 2 km after two days in either simulation.

Following salinity and dye simulations, simulations were made of bacterial concentrations. For these simulations, an extreme case was selected assuming raw sewage with no disinfection was discharged continuously over the 30 day period of simulation. Simulations were first conducted assuming that there was no die-off (treating bacteria as a conservative constituent) and then using representative die-off rates. The results of these simulations are provided in Figures 6-16 to 6-20 as averages over the period of simulation. The averages are compared to the minimum and maximum over the period of simulation at each model segment as well as to the standard deviations of the bacterial concentrations. Figures 6-16 and 6-17 illustrate results assuming that bacteria act conservatively, while Figures 6-18 and 6-19 illustrate projections assuming a die-off rate of 1.0 day^{-1}. A comparison of the monthly averaged concentrations for several die-off rates is provided in Figure 6-20.

The results of these simulations indicate that a moderate die-off rate would probably reduce bacterial concentrations below the criteria of 70 counts/100 ml outside of the buffer zone, extending 2 km both above and below the sewage outfall. However, if die-off was occurring at low rate, acceptable concentrations could easily be exceeded, as demonstrated where the bacteria were assumed not to die-off (act conservatively). More probably, the additional contamination observed is due to non-point sources. This analysis did not consider near-field effects or the possibility of bacterial resuspension from sediments, which should be considered before determining the appropriate enforcement and/or allocation action. Additionally, this application considered a flow regime over a single month. Additional simulations, with collection of supporting field data, may be required for critical environmental conditions to evaluate model performance and estimate variations in bacterial populations.

6.4.2. Example 2 - DO in a One-Dimensional Estuary

This second WASP4 example is for a simple branching estuary considering DO depletion. Given the nature of

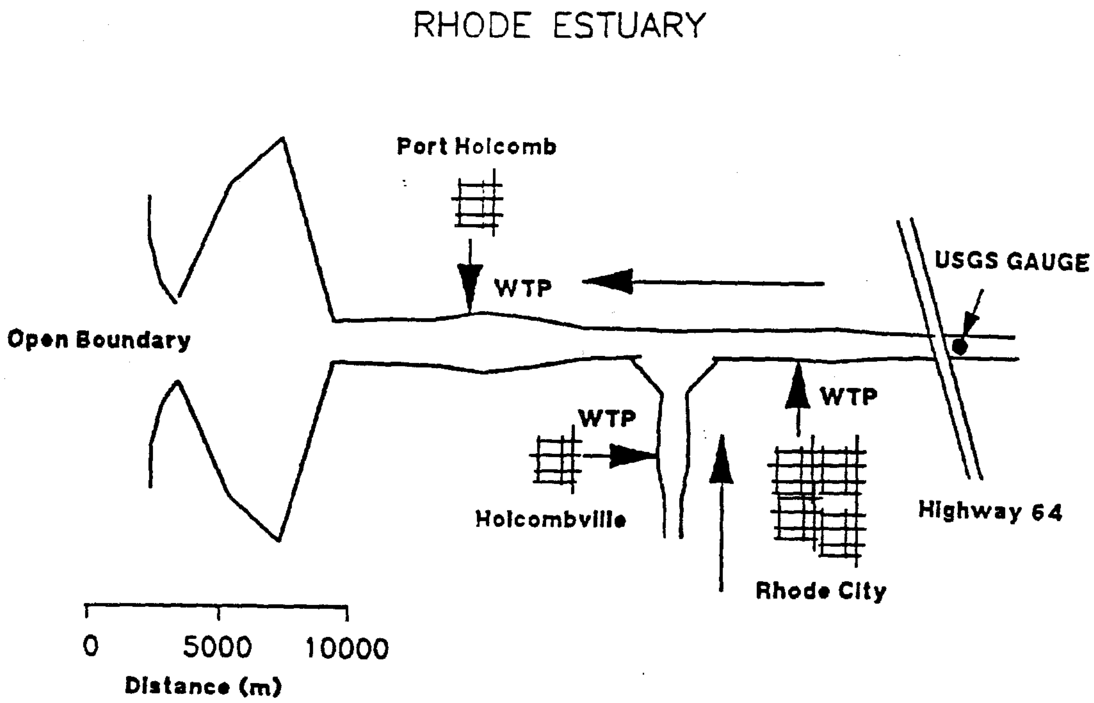

Figure 6-21. Morphometry of the Rhode Estuary.

the pollution problem, the eutrophication kinetic subroutine (EUTRO4) is required. The water quality variables of concern consist of DO, CBOD, and nitrogenous BOD. Water quality processes simulated include reaeration, sediment oxygen demand, nitrification and deoxygenation of CBOD.

This level of kinetic complexity has been extremely popular for simulating DO and the impact of oxygen demanding substances. Model calibration will consist of specification of the nitrification rate, CBOD deoxygenation rate, and reaeration rate. WASP4 provides the option of internally calculating the reaeration rate as a function of water depth and velocity. The reaeration rate will be manually specified for these simulations as model hydrodynamics are based upon tidal averaged conditions.

6.4.2.1. Problem Setting

In this example, three dischargers have been identified to the Rhode Estuary, including the city of Rhode, the town Holcombville, and Port Holcomb. The Holcombville WWTP discharges to Holcomb Creek, a tributary of the Rhode Estuary, while the Rhode and Port Holcomb WWTP discharge to the mainstem estuary. The city of Rhode is presently considering upgrading their WWTP to provide additional capacity. The city of Rhode is presently out of compliance for oxygen and proposes a modification of the existing plant to provide additional capacity and to come into compliance. The purpose of this example is to evaluate the proposed modifications. A summary of the problems setting and treatment plant data is presented in Figures 6-21 to 6-29 and Table 6-10.

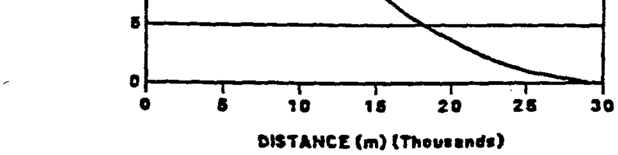

Figure 6-22. Mean salinity profile for the Rhode Estuary.

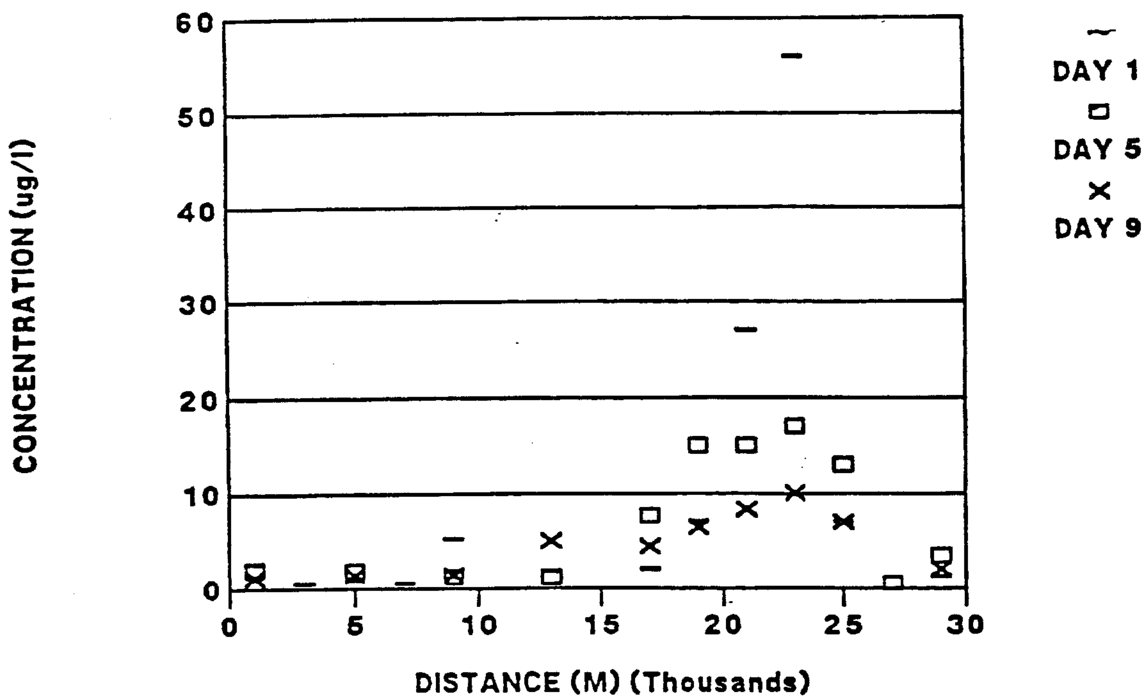

Figure 6-23. Results of the Rhode Estuary tracer study.

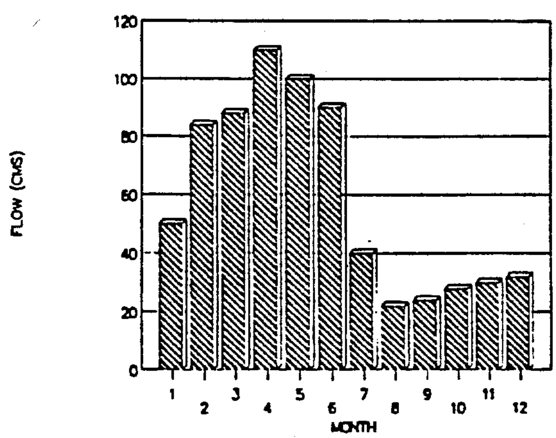

Figure 6-24. Average monthy flow at the Highway 64 USGS gauge.

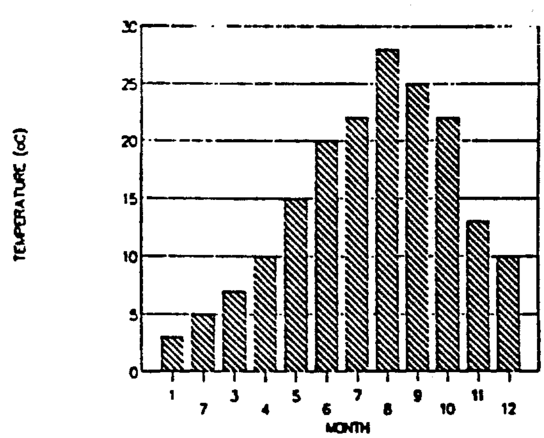

Figure 6-25. Mean monthly temperatures at the Highway 64 gauge.

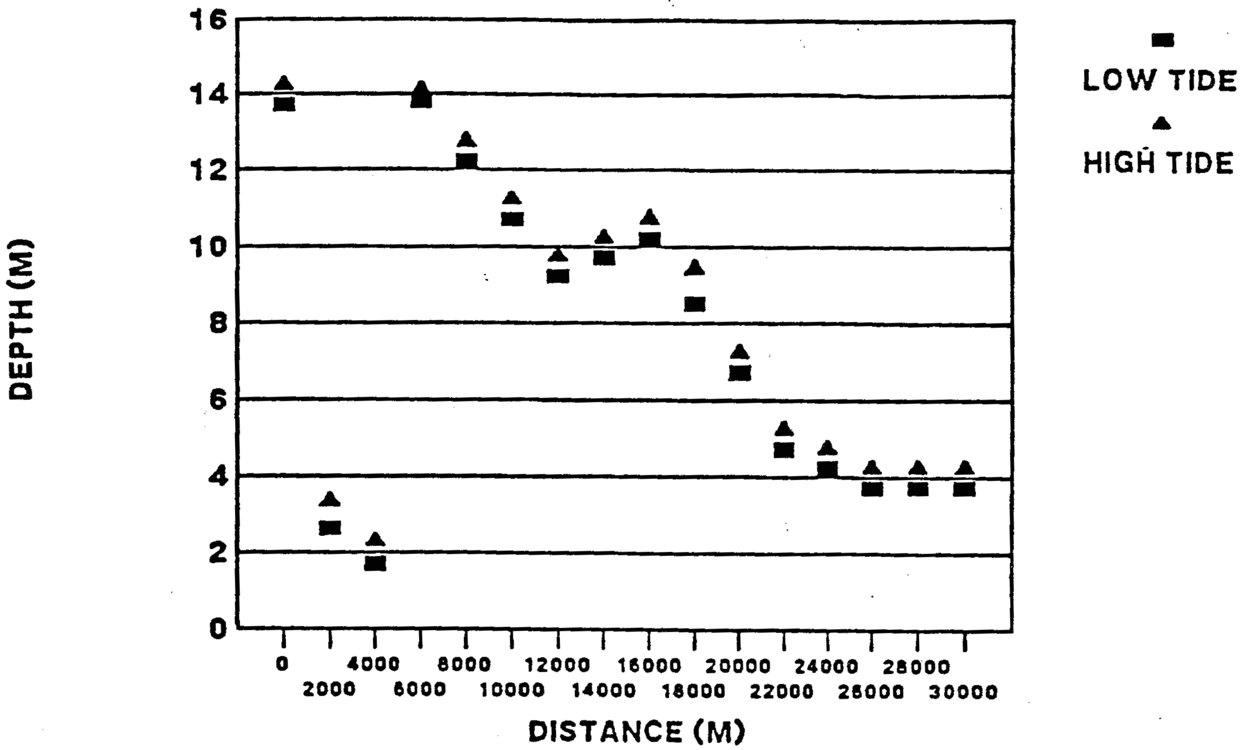

Figure 6-26. Mean depths for the Rhode Estuary versus distance upestuary from its mouth.

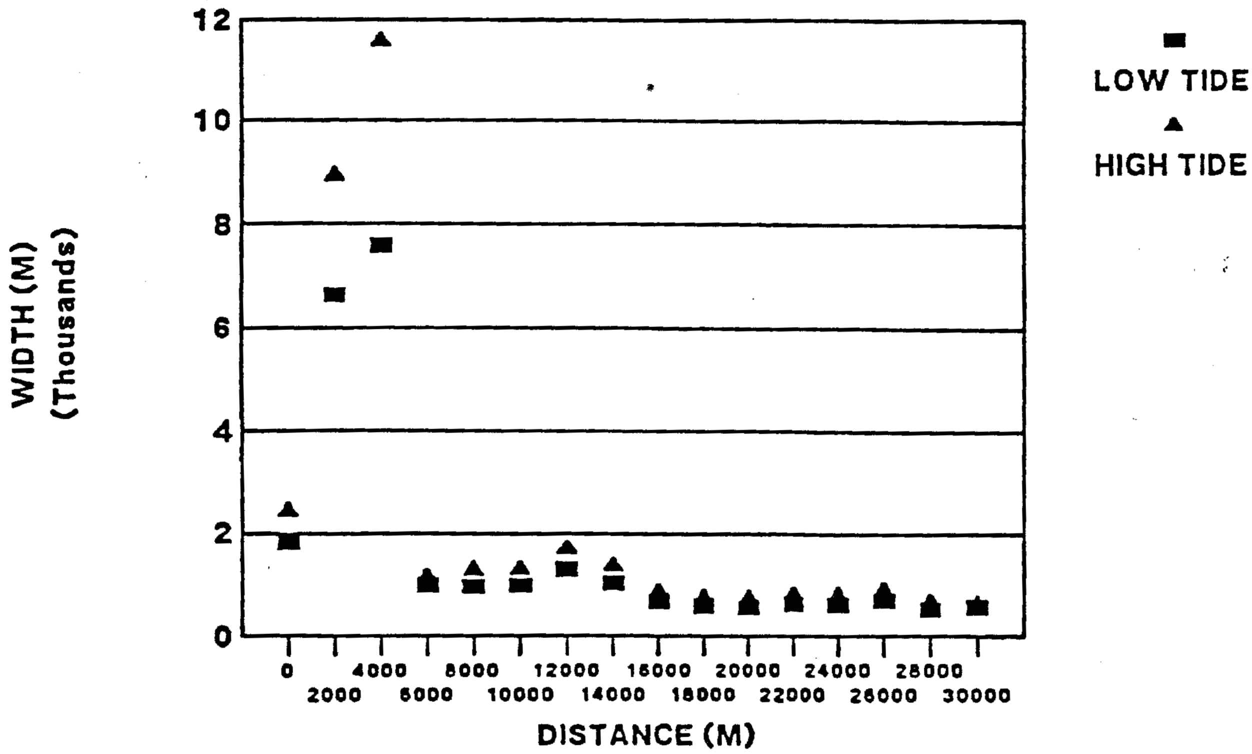

Figure 6-27. Mean widths of the Rhode Estuary versus distance upestuary from its mouth.

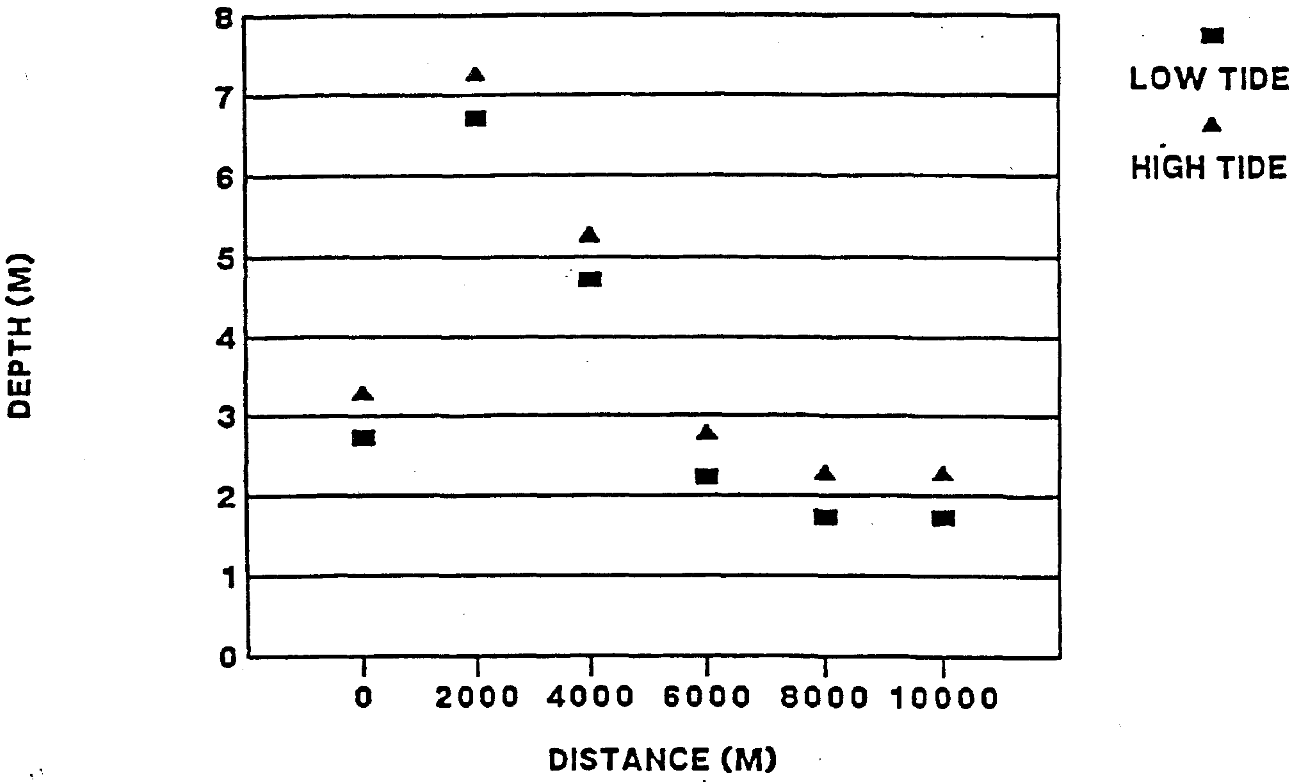

Figure 6-28. Mean depths of Holcomb Creek versus distance upstream from its mouth.

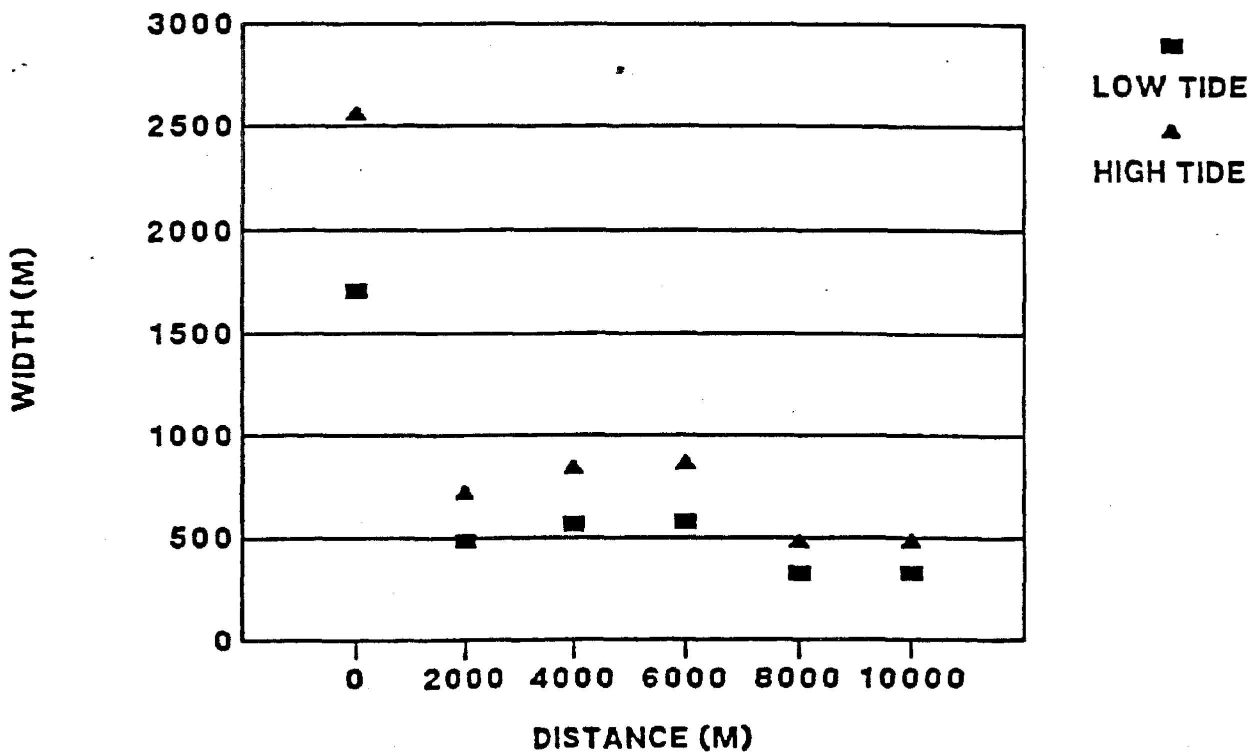

Figure 6-29. Mean widths for Holcomb Creek versus distance upstream from its mouth.

Table 6-10. Treatment Plant Effluent Characteristics

Rhode City WTP

Present: Trickling filter plant presently at capacity.
Proposed: Activated sludge plant.

		Present	Proposed
Flow	MGD	17	24
BOD_5	mg/L	60	30
$CBOD_u$ (1)	mg/L	120	60
NH_3-N	mg/L	30	20
DO	mg/L	5	5

(1) Based on long term BOD estimates of $CBOD_u/CBOD_5 = 2.0$

Holcombville

		Present
Flow	MGD	1.2
BOD_5	mg/L	65
$CBOD_u$ (1)	mg/L	130
NH_3-N	mg/L	40
DO	mg/L	5

Port Holcomb

		Present
Flow	MGD	0.48
BOD_5	mg/L	80
$CBOD_u$ (1)	mg/L	160
NH_3-N	mg/L	42
DO	mg/L	5

6.4.2.2. System Characteristics

The upstream section above the fall line is gauged by the USGS. The gauge is located near the crossing of Highway 64. The estuary has popular sport and commercial fisheries, including shellfish. The average monthly flows and temperatures taken at the USGS gauge are provided in Figures 6-24 and 6-25. The measured depths and widths at mean tide are provided in Figures 6-26 to 6-29. Mean tidal amplitude is 0.28 m. The pertinent water quality criterion is a minimum DO of 5.0 mg/l. From historical data, critical DO conditions occur in mid-August when the flow for the Rhode River at the USGS gauge is approximately 20 cms, and the Holcomb Creek (ungauged) flow is estimated to be 10 cms. Average August water temperatures is 27 °C.

6.4.2.3. Supporting Studies

Historical data within the study area were limited. Data were available for temperature at the USGS gauge. For this level of study, it was decided that an initial water quality survey would be conducted during the week of August 1. High and low slack measurements of DO, NH_3-N, BOD_5, and salinity were taken along the estuary and creek. The slack tide data were translated to mid-tide for comparison with the tidally averaged model. Flows during the study period for the Rhode River at the USGS gauge were approximately 20 cms, and the Holcomb Creek (ungauged) flows were estimated to be 10 cms, with averaged water temperatures of 27 °C at the USGS gauge. A single measurement near the USGS gauge indicated a BOD_5 of 0.7 mg/l in the Rhode River from that study. Two measurements of SOD were available, determined using an in-situ respirometer, from previous studies. A value of 1 g m^{-2} day^{-1} was measured in the lower estuary approximately 2 km above Port Holcomb and 2 g m^{-2} day^{-1} was measured approximately 1 km down-estuary of the Rhode WWTP discharge. A dye study was conducted with Rhodamine WT injected as a slug near the Rhode City WWTP discharge. The results of the dye study were used to evaluate model performance.

6.4.2.4. Model Application

This example requires similar information as the previous WASP4 example, with the exception of pollutant kinetics. However, it was elected not to use a hydrodynamic model for this application. Instead, simulations of tidally averaged conditions were conducted. Model inputs are described in detail in the Appendix available from the Center for Exposure Assessment Modeling, and are summarized below:

- General model information: Given the nature of the pollution problem, the eutrophication kinetic subroutine (EUTRO4) is required for this example. The water quality variables of concern consist of DO, CBOD, and nitrogenous BOD. Water quality processes simulated include reaeration, sediment oxygen demand, nitrification and deoxygenation of CBOD.

- Model Network: Analysis of the monitoring data indicated significant longitudinal gradients, with small lateral and vertical variations, allowing application of a one-dimensional model. A network was established consisting of 15 segments in the Rhode Estuary and 5 segments in Holcomb Creek. The variations in bottom morphometry and water quality were reasonably regular, and for simplicity segments were delineated every two kilometers. The depths of the segments were determined as well as segment volumes and interfacial areas from available morphometry data. The resulting network is illustrated in Figure 6-30.

- Dispersion coefficients: These coefficients are required to describe tidal mixing between all model segments. Initial estimates can be

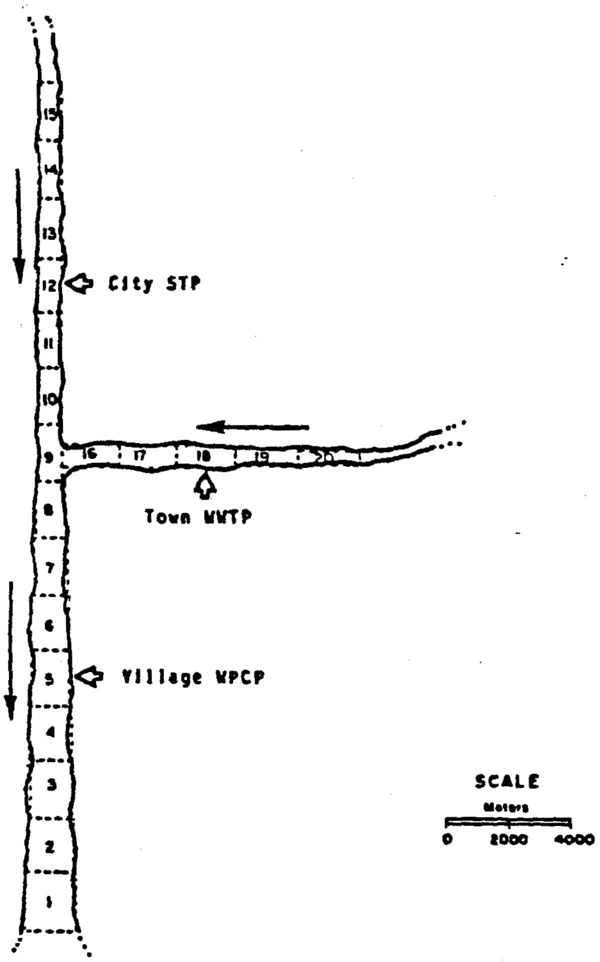

Figure 6-30. Model segmentation for the Rhode Estuary.

derived from the literature and refined through calibration to dye or salinity data. Their determination is described below.

- Segment volumes: The initial volume of each segment is required, as well as a description of how the volume changes with flow. Volumes were determined from segment width and depth (taken from hydrographic maps) and segment length (user specified).
- Flows: Net river flows during the survey period were 20 cms for the Rhode River and 10 cms for Holcomb Creek.
- Boundary concentrations: Boundary concentrations are required for CBOD, NBOD, and DO at segments 1, 15 and 20 (ocean and tidal river boundaries).
- Pollutant loads: Loading rates are required for CBOD, NBOD, and DO for each point source (WWTP and tidal rivers).
- Model parameters: Specification of salinity, temperature and sediment oxygen demand distribution both spatially and temporally.
- Model constants: Nitrification rate, CBOD deoxygenation rate, and reaeration rate.
- Initial concentration: Concentrations of CBOD, NBOD, and DO in each model segment are required for the beginning of the simulation. However, where simulations are conducted until steady-state is achieved, initial conditions are irrelevant.

6.4.2.5. Model Simulations

Simulations were first conducted for salinity and the dye tracer in order to evaluate predicted transport. To simulate steady-state salinity distribution using EUTRO4, the CBOD system was used with no decay specified (treated as a conservative material). Boundary conditions were established for salinity and initial conditions were set to zero. Simulations were then conducted until a steady-state salinity distribution was achieved.

The exchange coefficients in this example were estimated first from the salinity profile, indicating a dispersion rate of approximately 30 m^2 sec^{-1}. Boundary flows and concentrations were input, with 30 ppt as the ocean boundary, and simulations were conducted for a period of 50 days using constant boundary conditions. The 50-day period was selected as sufficient for the predicted concentrations to reach steady-state for comparison with field data. Simulations indicated that a constant exchange coefficient of 22 m^2 sec^{-1} allowed reasonable representation of the salinity distribution. A comparison of model predictions and field data for different exchange coefficients is provided in Figure 6-31.

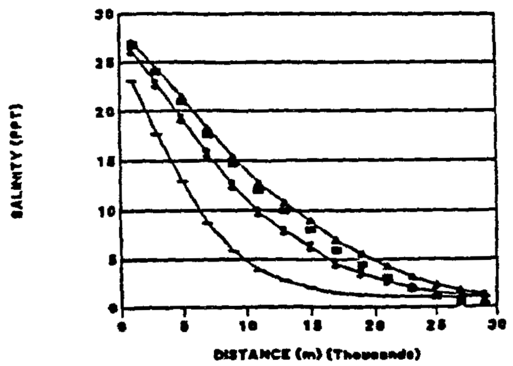

Figure 6-31. Comparison of predicted and observed salinities for different values of the dispersion coefficient.

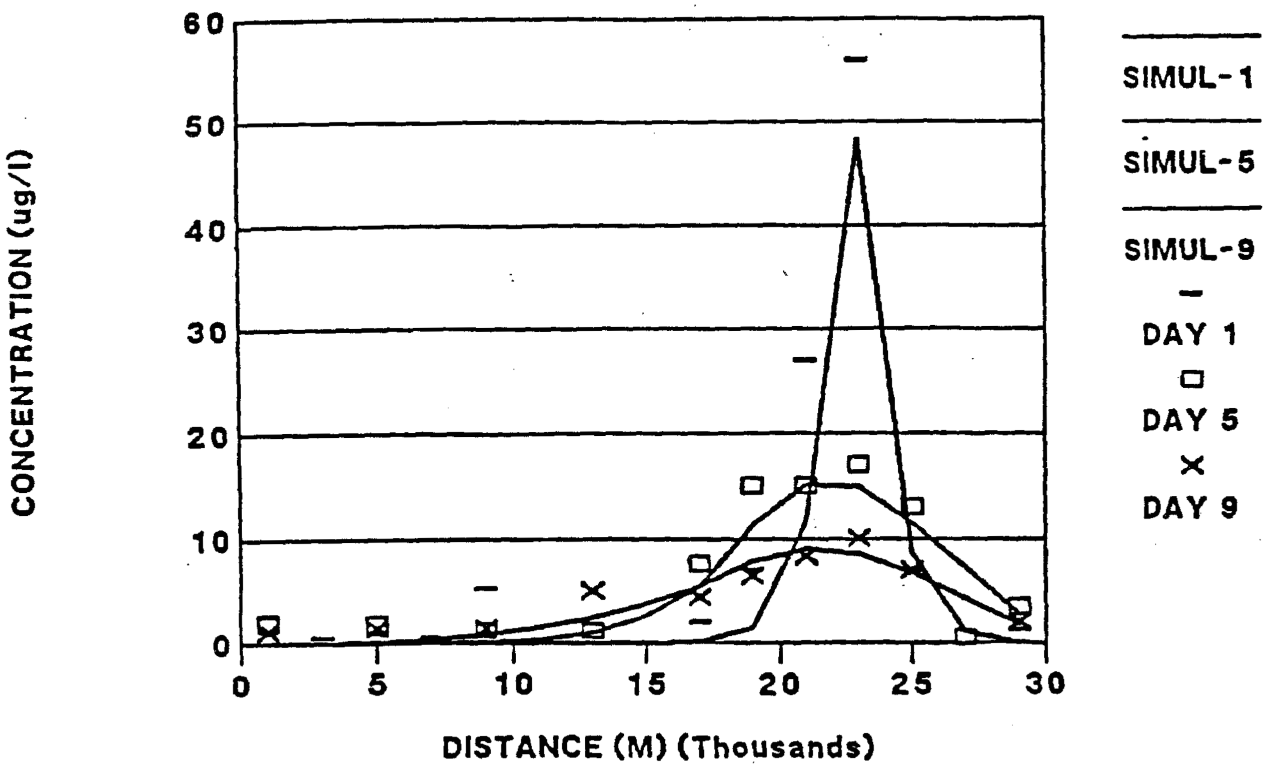

Figure 6-32. Comparison of measured and observed dye concentrations.

Beginning August 1, in conjunction with other water quality surveys, a dye study was conducted. Rhodamine WT was injected in the effluent of the Rhode City WTP. The dye density was adjusted with alcohol to avoid sinking, and a steady concentration of 8 mg/l was maintained in the effluent over one complete tidal cycle. This 8 mg/l concentration in the effluent was calculated to provide a completely mixed concentration of approximately 100 ppb in the Rhode Estuary near the point of discharge. Monitoring continued for 8 days following the discharge. High and low slack data were obtained and processed to provide tidally averaged concentrations. As with salinity, the dye was simulated using the CBOD system and treating it as a conservative material. Boundary concentrations were set to zero and loadings of dye were specified with a duration of 12.5 hours. Since the model had been previously calibrated using salinity data, the dye data were used to evaluate model performance. The predicted and observed concentrations are compared in Figure 6-32, and as illustrated, the simulations were considered acceptable.

Following evaluation of the simulations of salinity and the dye tracer, simulations were conducted for NBOD, CBOD, and then DO. This sequence results from NBOD and CBOD being unaffected by DO (if DO does not approach zero), while DO is affected by these parameters as well as SOD and reaeration. Therefore, simulations proceed from the simple to the complex.

Simulations were conducted first using literature values for the nitrification rate and CBOD deoxygenation rate. It was elected to specify a reaeration rate rather than use model formulations to calculate a rate, because reaeration rates had been measured in the vicinity under similar conditions. The salinity, SOD and temperature were specified in the model parameter list. The SOD was assumed to be 2.0 g m^{-2} day^{-1} in the vicinity of the Rhode WWTP and 1.0 elsewhere. Simulations were conducted with varying nitrification and deoxygenation rates. Field data and model predictions are compared in Figures 6-33 to 6-36. While no statistical analyses were performed, visual inspection indicated that model predictions were adequate for this study.

6.4.2.6. Model Predictions

Once reasonable predictions were obtained, simulations were conducted projecting DO, NBOD and CBOD concentrations in the estuary following implementation of the proposed modifications at the Rhode WWTP (Table 6-10, see Figure 6-37). These simulations suggested that little change would be expected in the DO concentrations as a result of the proposed modifications.

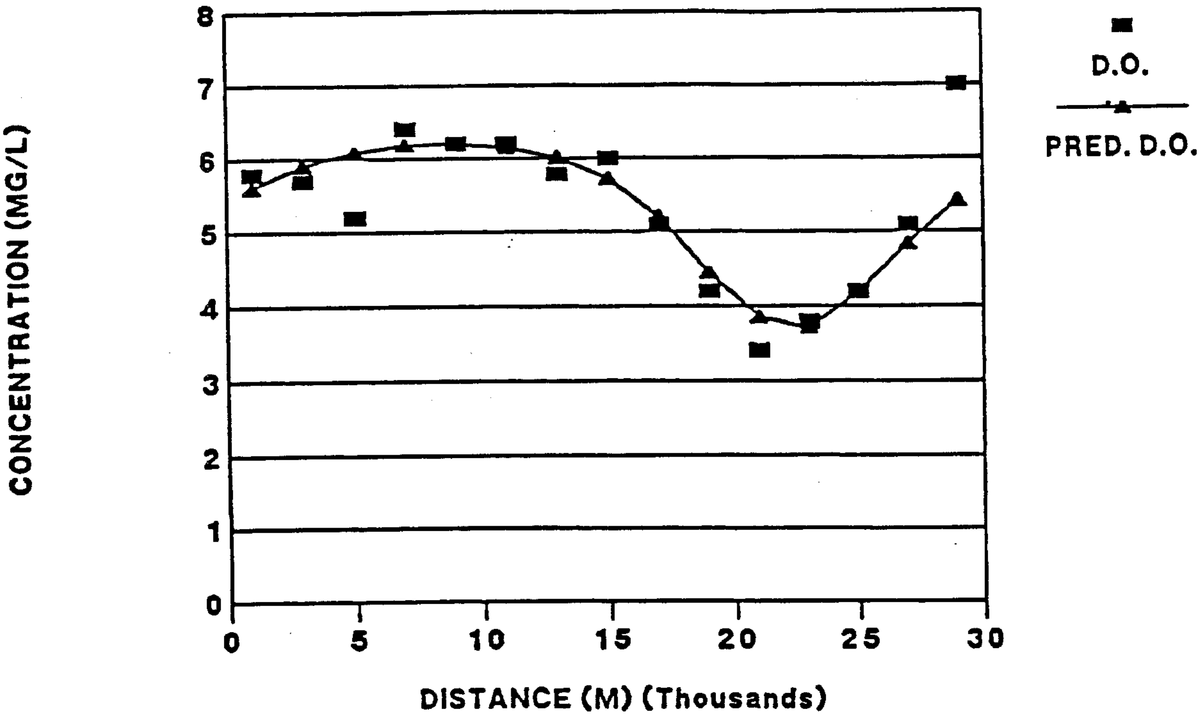

Figure 6-33. Measured and predicted DO concentrations in the Rhode Estuary versus distance upestuary from its mouth.

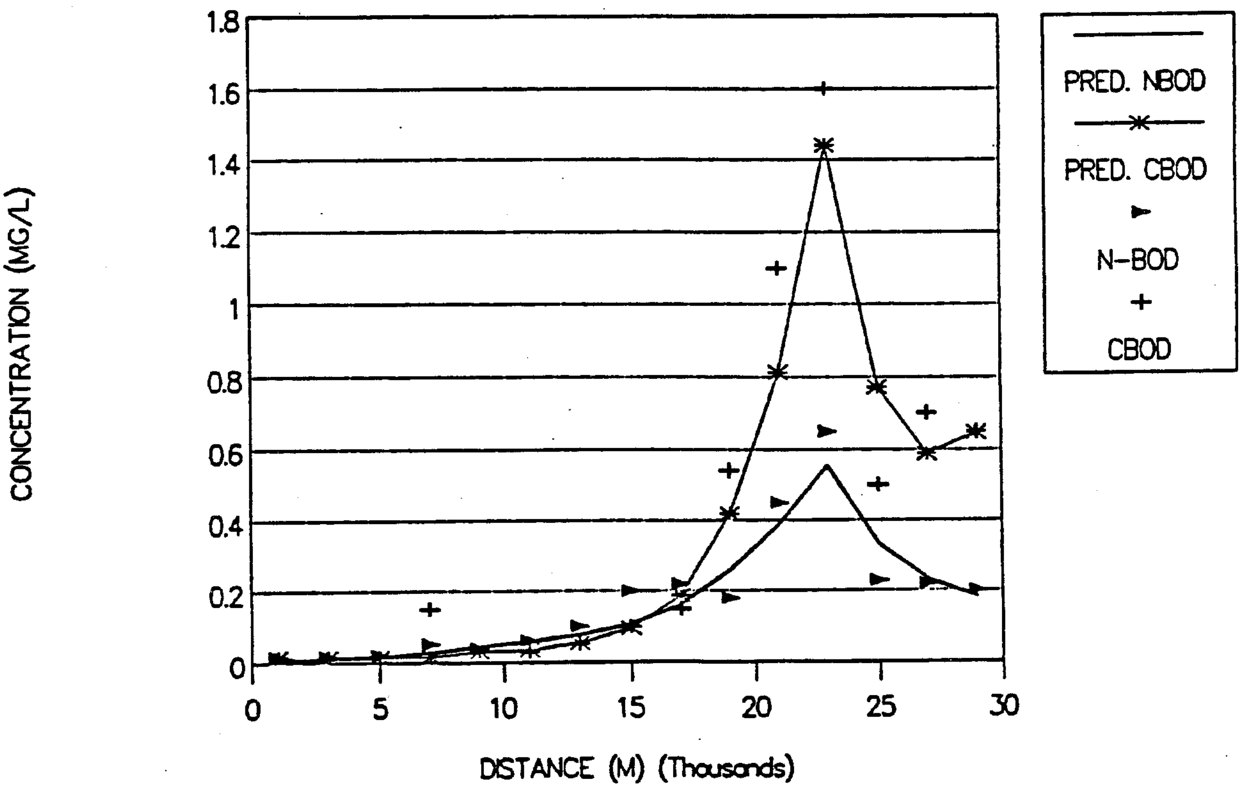

Figure 6-34. Predicted and observed NBOD and CBOD concentrations in the Rhode Estuary versus distance upestuary from its mouth.

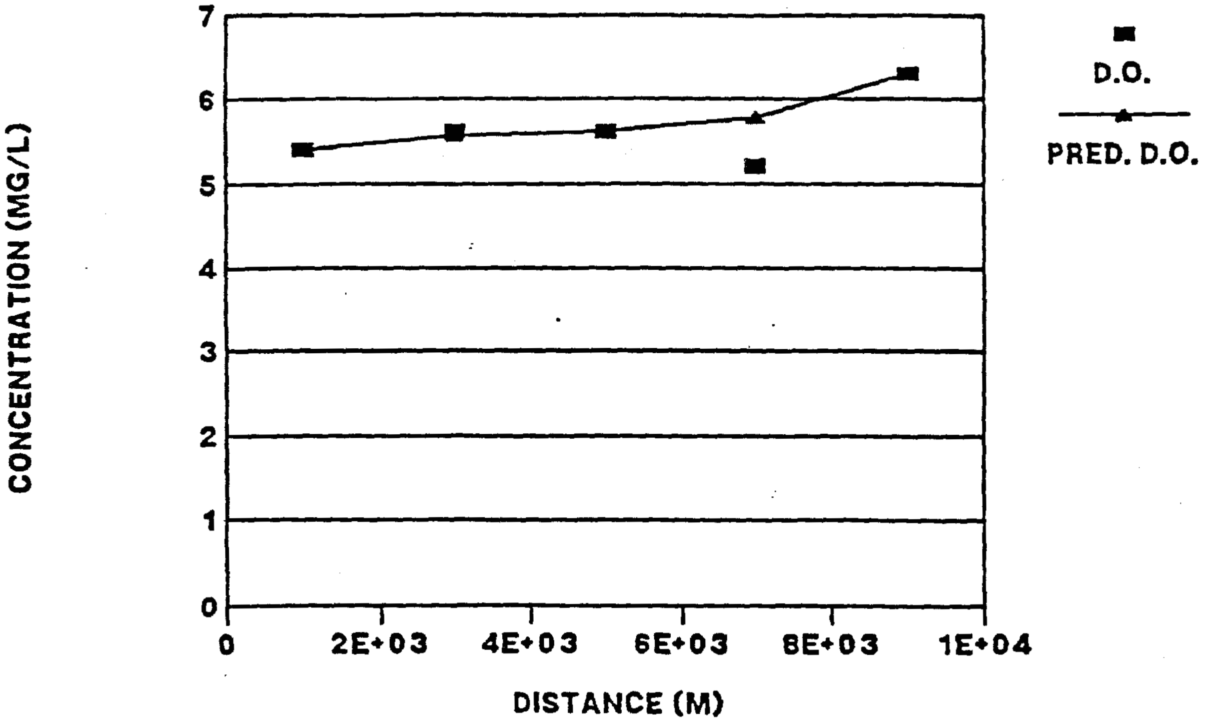

Figure 6-35. Predicted and observed NBOD and CBOD concentrations in the Rhode Estuary versus distance upestuary from its mouth.

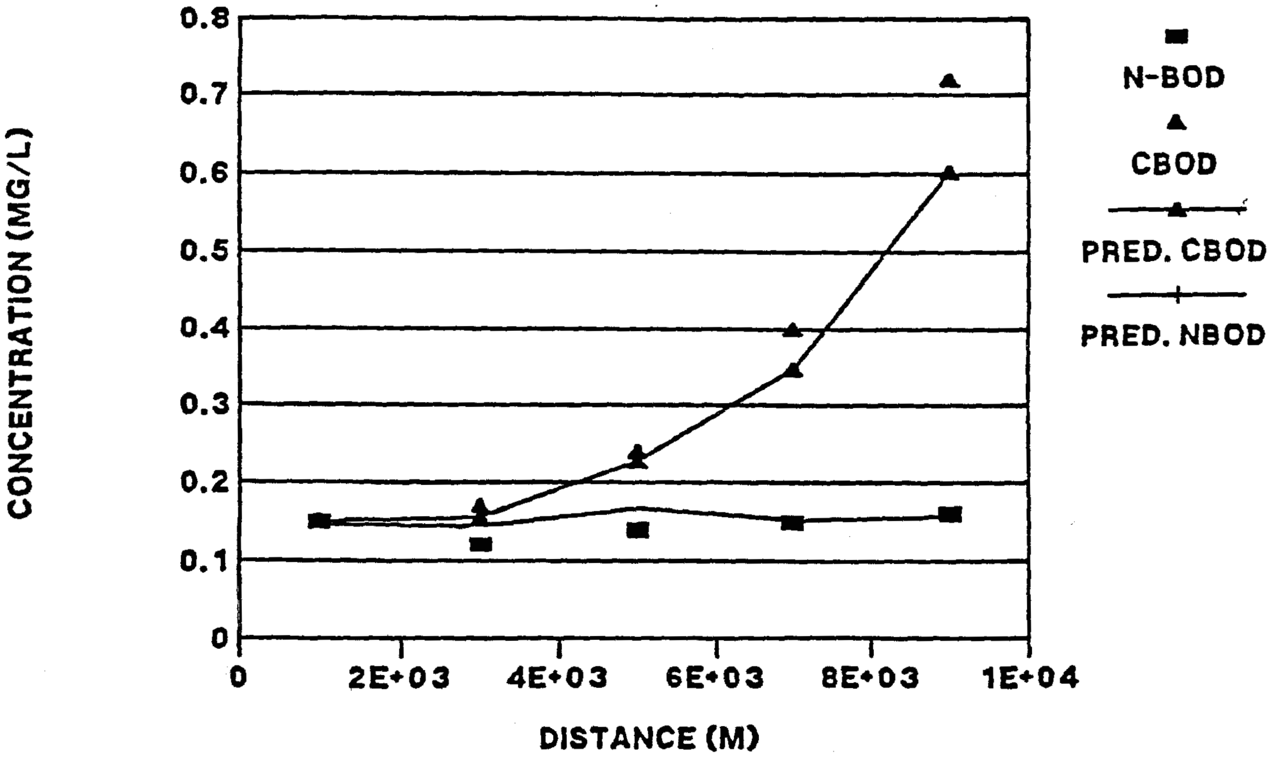

Figure 6-36. Measured and predicted DO concentrations in Holcomb Creek versus distance upstream from its mouth.

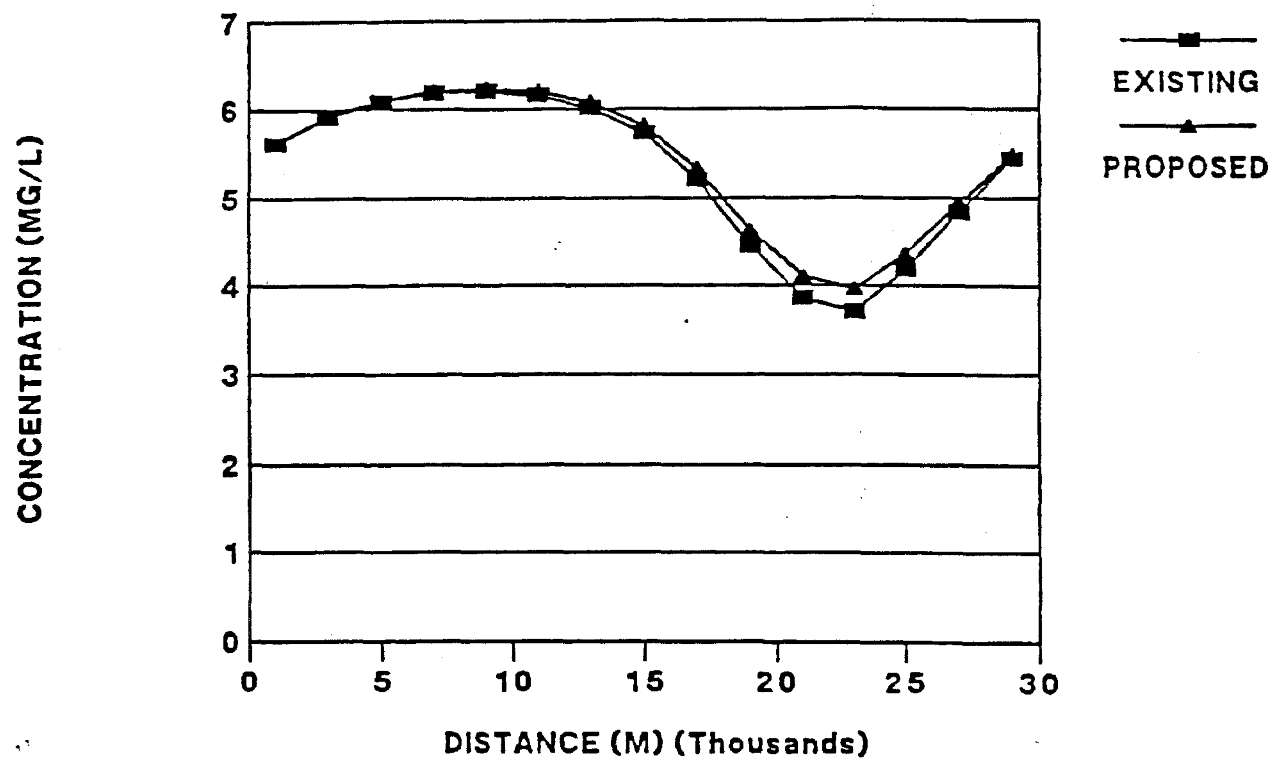

Figure 6-37. Comparison of DO predictions under existing and proposed conditions for the Rhode City WWTP.

The final waste load allocation should not result from a single model projection. The model should be evaluated using independent data, if possible. A component analysis should be performed to determine the relative contributions of SOD, reaeration, CBOD and NBOD to the DO concentrations. The component analysis may provide information which would be useful in project design. Sensitivity analyses should also be performed to determine the effects of assumptions concerning the selection of model parameters. Consideration should also be given to the applicability of calibrated rates to future conditions. Examples include CBOD deoxygenation and nitrification rates and sediment oxygen demand, which can decrease under future conditions where improved wastewater treatment occurs. The tested model can be used to estimate the reduction in waste load required to meet water quality objectives.

Port Holcomb was clearly in violation of its permit, discharging essentially raw wastewater into the estuary. However, as a result of its advantageous location, its discharges seemed to have little impact on DO concentrations, when averaged over the estuarine cross-section. Additional field and modeling work is required to identify the extent of the problem. However, as a result of the bacteriological problem that has resulted, permit/enforcement action is pending which would impact its BOD release as well.

6.4.3. Example 3 - Nutrient Enrichment in a Vertically Stratified Estuary

The third and fourth examples apply to a vertically stratified estuary. This type of estuary has significant differences in water quality both longitudinally and with depth. Estuary widths are still narrow enough that lateral variations in water quality are not important; vertical stratification is such, however, that the water column must be divided into discrete vertical layers. This type of characterization typically occurs in deeper estuaries or in areas characterized by a salinity intrusion wedge.

6.4.3.1 Problem Setting

The city of Athens, population 180,000, is located on the upper reaches of Deep Bay (Figure 6-38). This relatively deep estuary is driven by moderate 1 meter tides and a large but seasonably variable inflow from Deep River, which is gauged above the fall line. The seaward reaches of Deep Bay are used for both commercial fishing and shellfishing, and the upper reach is spawning habitat. Boating and recreational fishing are popular, as are several bathing beaches. Pertinent

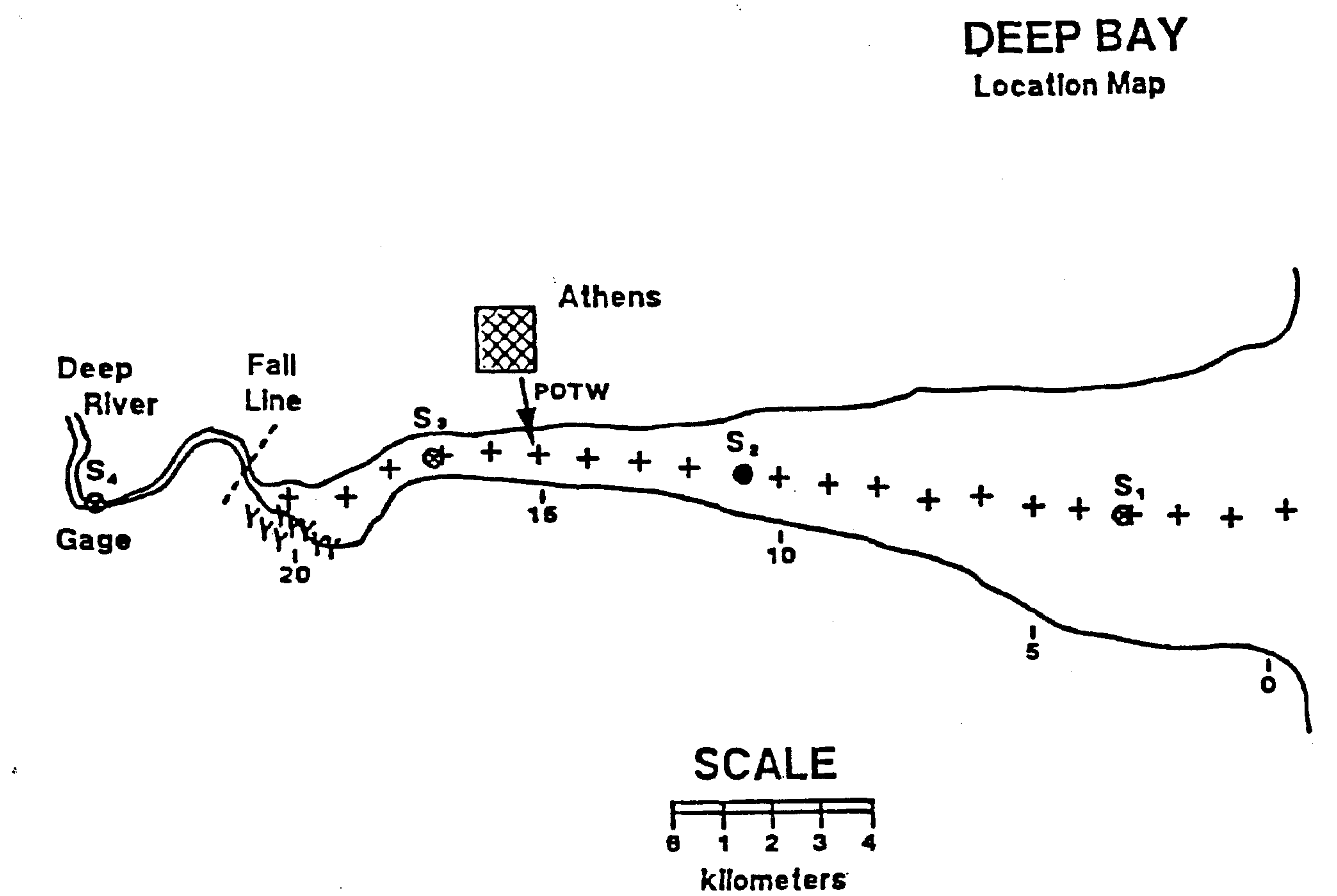

Figure 6-38. Deep Bay location map.

criteria and water quality goals are 5.0 mg/L for DO and 25 μg/L chlorophyll a.

Athens is maintaining a poorly operated secondary wastewater treatment plant that discharges from a surface pipe near shore 15 km from the mouth of Deep Bay. Periodic episodes of low benthic DO near the discharge and moderate phytoplankton blooms downstream have been occurring. Renovation of the plant to high performance secondary or possibly tertiary treatment is being considered, as are point and nonpoint source controls in the watershed.

Bathymetric surveys have produced a chart of soundings at low tide, used for navigation (Figure 6-39). Surveys were conducted in April, June, and August to characterize tide, salinity, temperature, and light transmittance. Continuous velocity and salinity data were obtained from moorings at S1, S2, and S3 over these three five-day periods (Tables 6-11and 6-12). Deep River flow data are summarized as monthly averages, and the observed range of water quality constituents is tabulated in Table 6-13. A study on the upper watershed has produced estimates of these water quality constituents under a program of nonpoint source watershed controls. A study of the Athens POTW has produced average quality for the present effluent, and estimates were made of effluent quality expected following possible plant upgrading (Table 6-14).

Table 6-11. Summary of Deep Bay Tidal Monitoring Data

			Rms Velocity[2]		Net Velocity[2]	
Station	Date	Tidal Range[1]	Surface	Bottom	Surface	Bottom
S1	4/19-23	0.9	340	260	+2.1	+0.2
(km 3)	6/13-17	1.0	350	260	+0.6	+0.0
	8/14-18	0.9	330	260	+0.2	-0.0
S2	4/19-23	1.1	370	270	+5.3	+0.7
(km11)	6/13-17	1.2	350	260	+1.4	+0.2
	8/14-18	1.1	350	250	+0.4	+0.0
S3	4/19-23	0.8	320	310	+10.4	+8.9
(km 17)	6/13-17	0.9	300	300	+2.8	+2.3
	8/14-18	0.8	290	280	+0.7	+0.6

[1] meters
[2] cm/sec

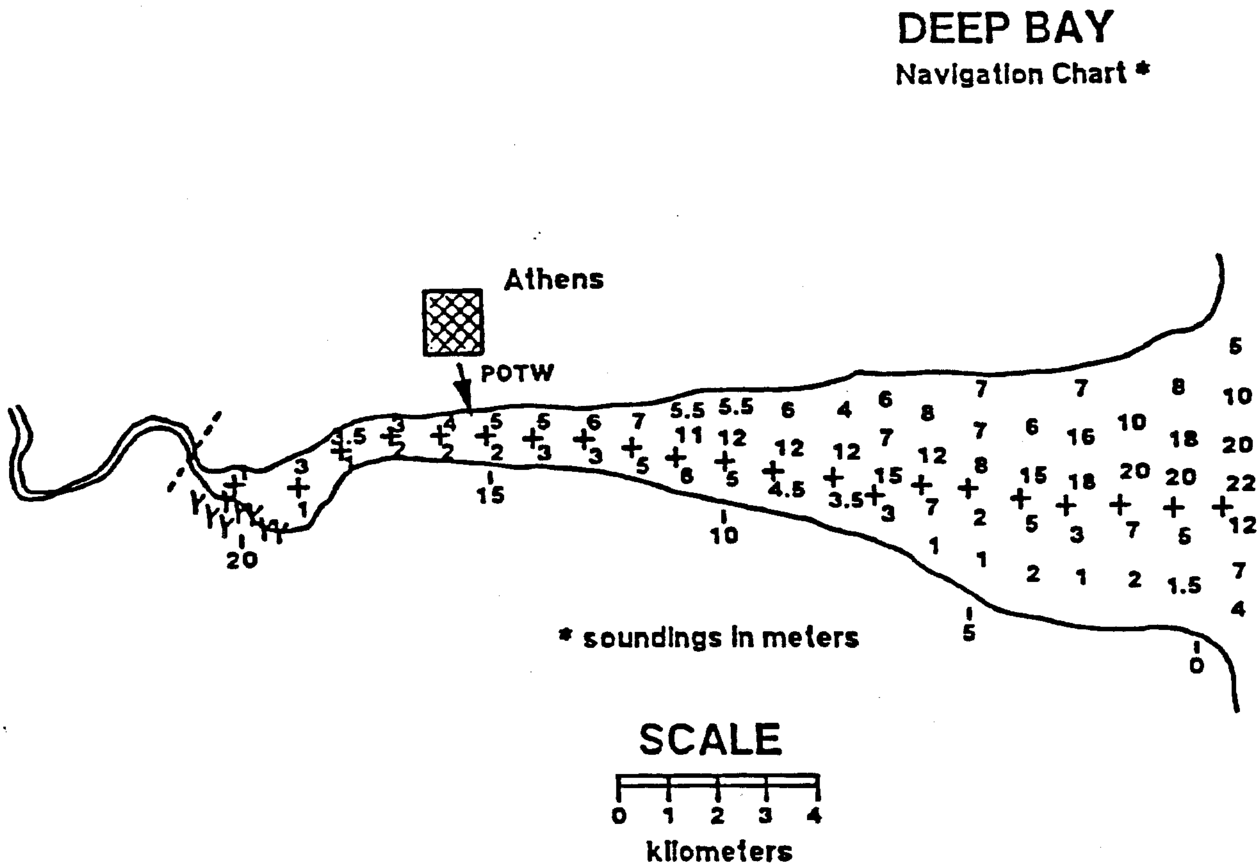

Figure 6-39. Deep Bay navigation chart.

Table 6-12. Summary of Deep Bay Estuarine Data

Station	Date	Salinity (kg/L) Surface	Salinity (kg/L) Bottom	Temperature (°C) Surface	Temperature (°C) Bottom	Secchi Depth (m)
S1	4/19-23	14.0	21.1	14	15	3.3
	6/13-17	22.5	24.5	23	22	2.7
	8/14-18	27.2	28.0	22	21	3.0
S2	4/19-23	15.7	15.5	15	17	1.7
	6/13-17	8.5	12.3	25	22	1.3
	8/14-18	19.5	21.8	23	22	1.5
S3	4/19-23	0.1	0.3	16	18	0.7
	6/13-17	1.0	3.1	26	23	0.5
	8/14-18	9.1	10.7	24	22	1.0

Table 6-14. Summary of Athens POTW Effluent Data

Design Capacity - 60 MGD
Secondary Treatment, with problems

Alternative	DO	BOD_5	Nitrogen ORG	Nitrogen NH_3	Nitrogen NO_3	Phosphorus Org	Phosphorus PO_4
Present	4	40	15	15	0	3	7
Good Secondary	5	20	0	15	15	3	7
Tertiary	6	10	0	2	10	0	0.5

Table 6-13. Deep River Data

Monthly Flow (m^3/sec)

Month	Average	Survey Year	Month	Average	Survey Year
January	90	85	July	60	40
February	80	75	August	50	20
March	120	150	Sept	50	40
April	210	300	October	110	150
May	175	200	Nov	140	140
June	120	100	Dec	130	150

Water Quality (mg/l)

Constituent	Present Minimum	Present Maximum	Watershed Controls
TKN	0.1	0.4	0.02
ORG-N	0.0	0.3	0.01
Nitrate-N	0.3	0.6	0.10
Ortho-P	0.04	0.12	0.01
Organic-P	0.01	0.05	0.005
BOD_5	0.5	1.0	0.2
DO	5	14	7-14
SS	10	1000	10-250

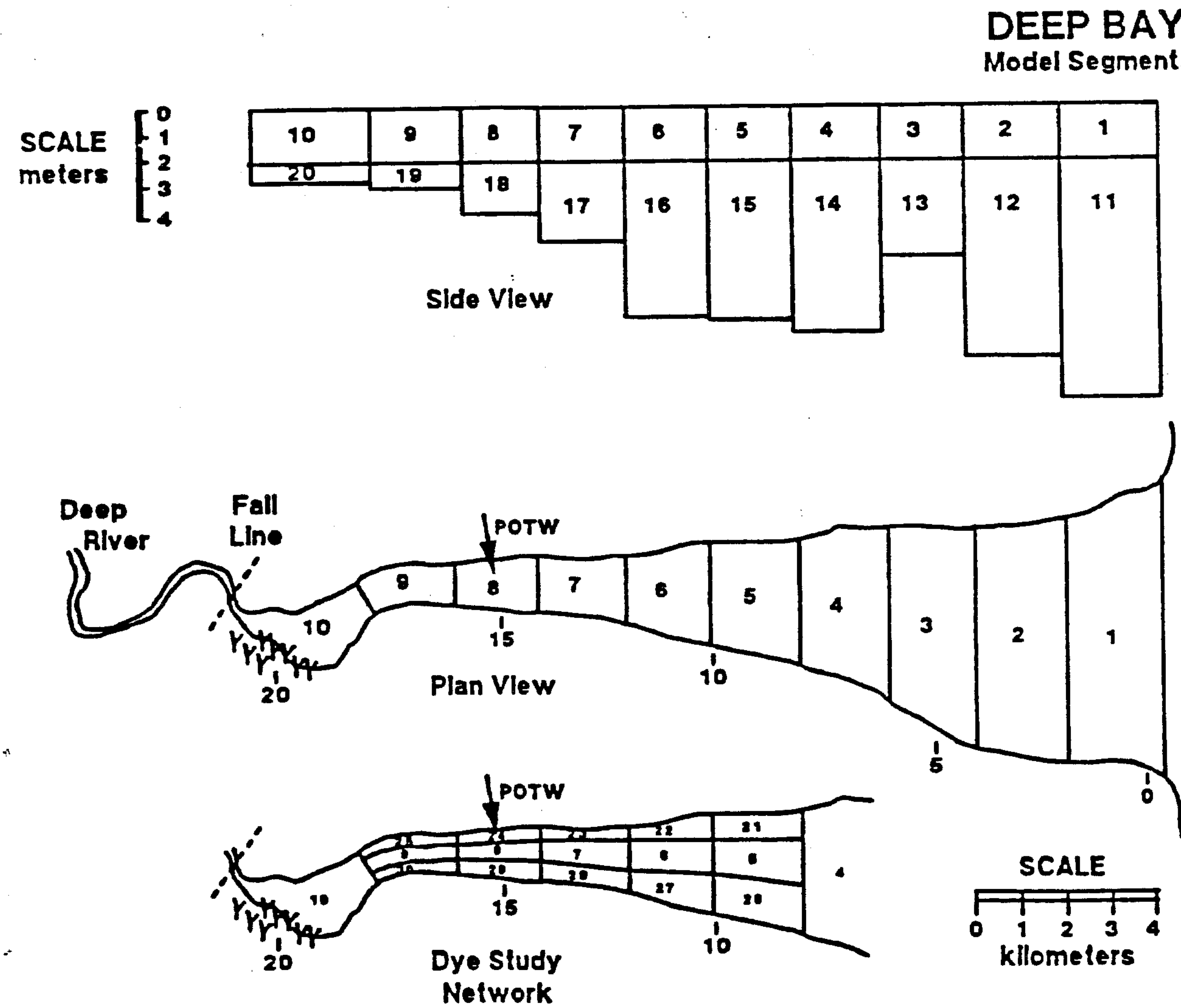

Figure 6-40. Deep Bay model segmentation.

6.4.3.2 Deep Bay Network

Analysis of the monitoring data show significant differences between surface and bottom mean velocity and salinity, indicating a partially mixed estuary. Because of these vertical variations and because bottom water DO was reported to be low, a 2 dimensional x-z network was chosen. For convenience, segments were delineated every 2 kilometers, giving 20 water column segments with 2 vertical layers of 10 segments each. Surface water segments are a uniform 2 meters in depth, while underlying water segments range from 10 meters near the mouth to 0.5 meters upstream. The resulting network is illustrated in Figure 6-40.

6.4.3.3 Deep Bay Salinity

Simulation of salinity allows calibration of dispersion coefficients and density currents. Information needs are as follows:

- General model information: One system is simulated - system 1 is interpreted as salinity, and systems 2-8 are bypassed. The simulation begins on day 21, representing the April 21 survey, and ends on day 147, a week following the August 11 survey.
- Dispersion coefficients: This estuary requires two types of dispersion coefficients - longitudinal dispersion (representing tidal mixing) and vertical eddy diffusion.
- Segment volumes: Mean tide volumes are specified for all surface and subsurface segments.
- Flows: Tributary flow is partitioned to surface and bottom segments and routed through the estuary. Monthly river flows are specified. A density flow from the ocean is routed upstream

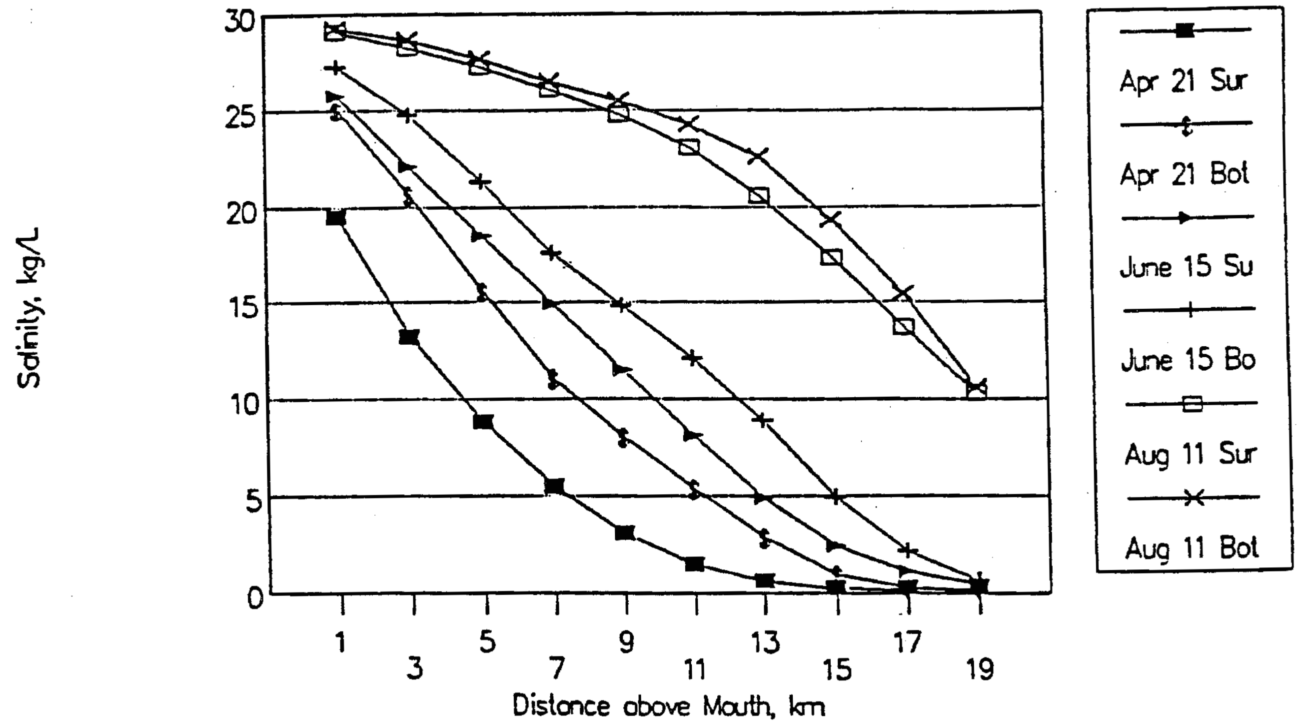

Figure 6-41. Deep Bay salinity Apr-Aug mean response.

along the bottom with vertical entrainment and downstream flow along the surface.

- Boundary concentrations: A constant downstream concentration of 30 mg/L was assumed. Upstream salinity concentrations are set to 0.
- Pollutant loads: No loads are input.
- Environmental parameters: No parameters are input.
- Kinetic constants: No constants are needed.
- Environmental time functions: No time functions are needed.
- Initial concentrations: Initial salinity concentrations are assigned each segment based upon an April survey. Dissolved fractions are set to 1.0.

Analysis of the depth-averaged salinity data during the three monitoring periods indicates estuarine-wide dispersion from 20 to 50 m^2/sec. A constant value of 30 m^2/sec was assigned. The tributary inflow was partitioned 70% to surface and 30% to bottom layers. Analysis of bottom current data indicates that a net flow of approximately 10 m^3/sec enters the estuary along the bottom at the mouth. This bottom inflow was attenuated upstream, entraining a fraction to the surface to satisfy continuity and match surface and bottom salinity data. The salinity simulation began on the first day of the April survey, using survey results as initial conditions. The simulation continued through August, with water column concentrations printed out corresponding to the July and August surveys. Results are illustrated in Figure 6-41.

6.4.3.4 Deep Bay Dye Study

To better evaluate vertical and horizontal dispersion near the Athens outfall, a dye study was carried out. Information needs for the model are similar to those for salinity:

- General model information: One system is simulated - system 1 is interpreted as dye, and systems 2-8 are bypassed. The simulation begins on day 75, the day preceding the June 14 dye study, and terminates on day 110.
- Dispersion coefficients: The same longitudinal and vertical dispersion coefficients calibrated in the salinity simulation are used. The upstream portion of the network is divided into lateral segments, and lateral dispersion coefficients are required.

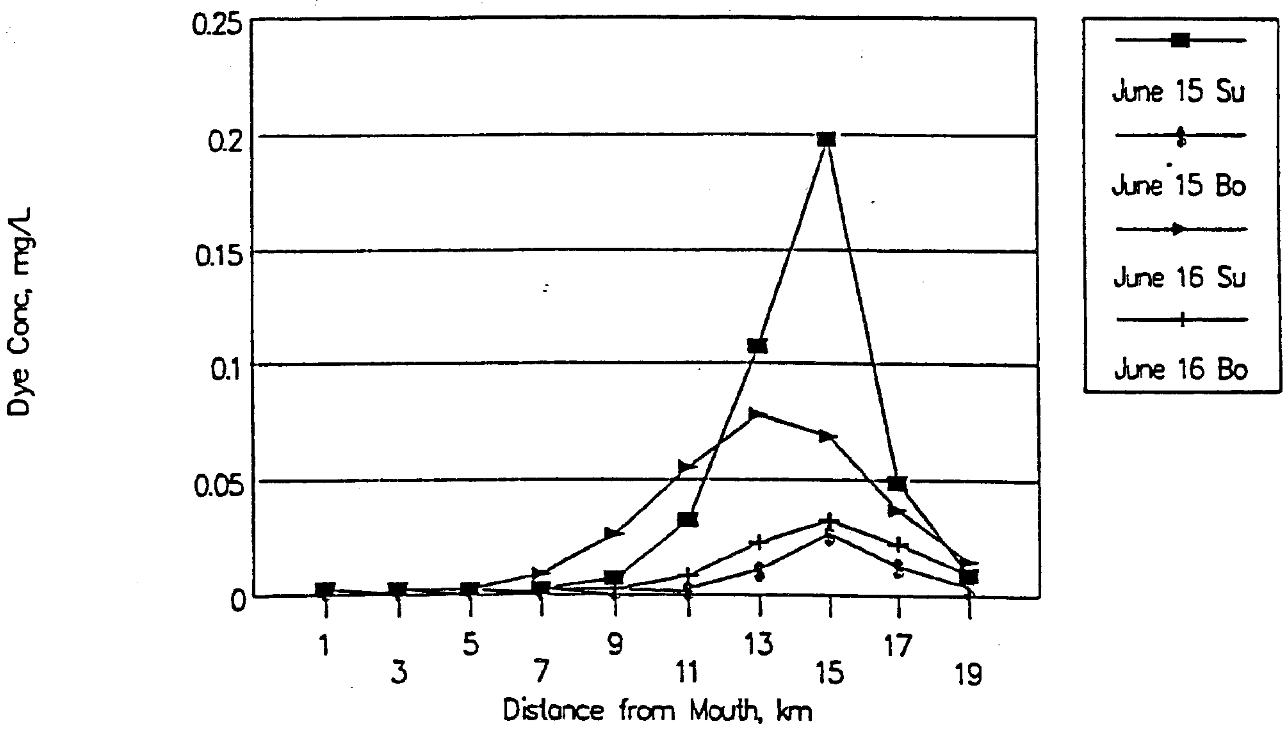

Figure 6-43. Deep Bay dye study center channel, surface and bottom.

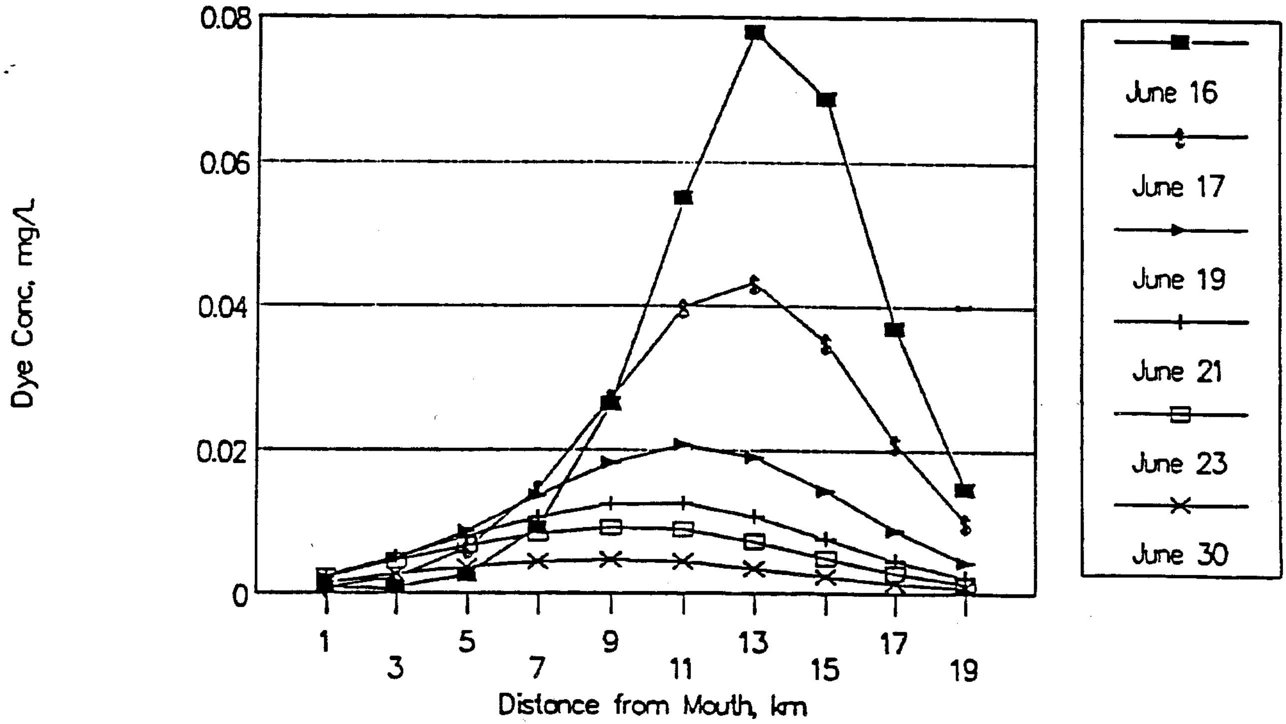

Figure 6-44. Deep Bay dye study center channel, surface.

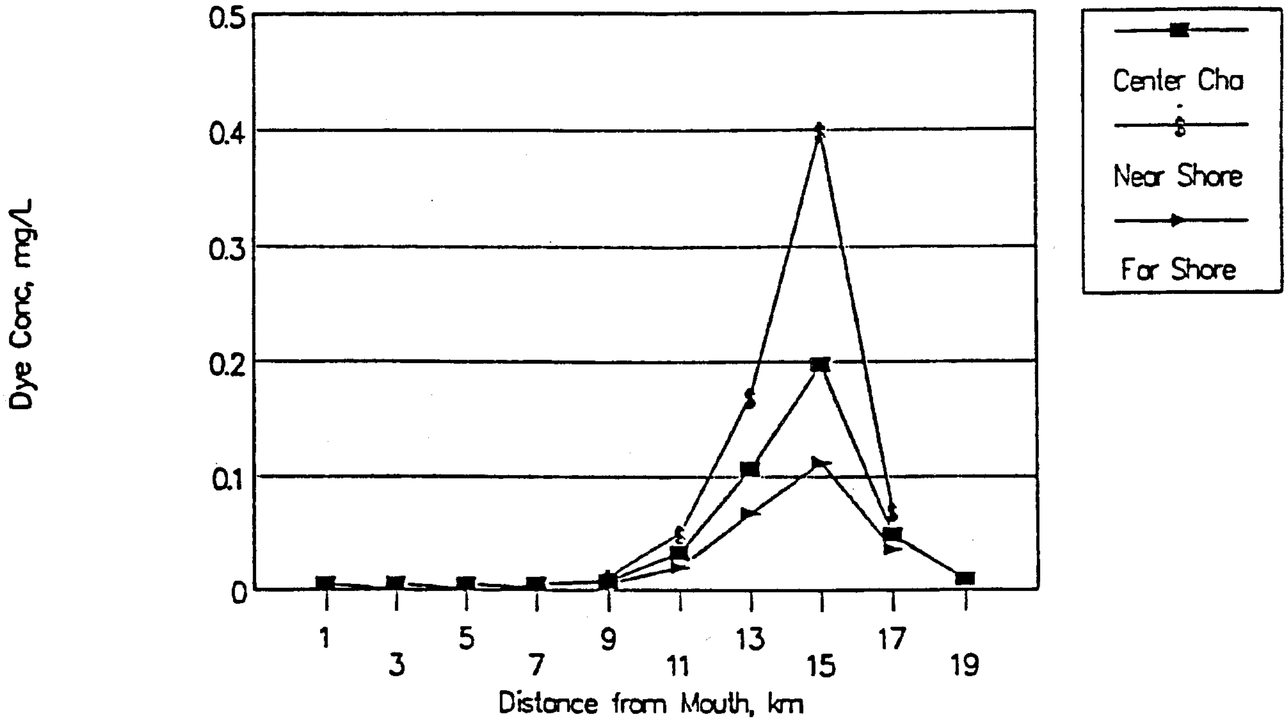

Figure 6-42. Deep Bay dye study June 15, surface.

- Segment volumes: The same mean tide volumes from the salinity simulation are used, except the upstream segments are divided into three for lateral resolution.
- Flows: The same flows from the salinity simulation are used, except the flow is partitioned laterally in the upper network.
- Boundary concentrations: Upstream and seaward boundary concentrations of 0 are specified.
- Pollutant loads: A one day load of dye is specified for the near shore surface segment adjoining the Athens POTW.
- Environmental parameters: No parameters are needed.
- Kinetic constants: One constant is specified - a low nitrification rate is entered, representing net loss of dye.
- Time functions: No time functions are needed.
- Initial concentrations: Initial concentrations of 0 are entered.

Beginning on June 14 (day 75), Rhodamine WT was metered into the 3 m^3/sec waste stream. A steady 10 mg/L concentration in the effluent was maintained for one day. High and low slack samples were taken daily for one week along the near shore, center channel, and far shore at both surface and bottom. The slack tide data were translated to mid-tide for comparison with the tidal-averaged model. The salinity network was modified for the dye study to calculate lateral mixing near the outfall (Figure 6-40). Vertical and lateral dispersion coefficients in the upper network were adjusted to best fit the dye profiles. Lateral and longitudinal variations in the surface layer after one day are shown in Figure 6-42. The lateral variations had virtually disappeared by the second day. Vertical and longitudinal variations in mid-channel after one and two days are shown in Figure 6-43. Mid-channel profiles for the first 2 weeks are shown in Figure 6-44. The model was judged sufficiently calibrated for estuarine-wide transport.

6.4.3.5 Deep Bay Total Nutrients

To evaluate eutrophication potential throughout Deep Bay, simulations of total nitrogen and phosphorus were conducted. Information needs are as follows:

- General model information: Two systems are simulated - system 1 is interpreted as total nitrogen and system 3 as total phosphorus. Systems 2 and 4-8 are bypassed. The simulation begins on day 1 (April 1) and terminates on day

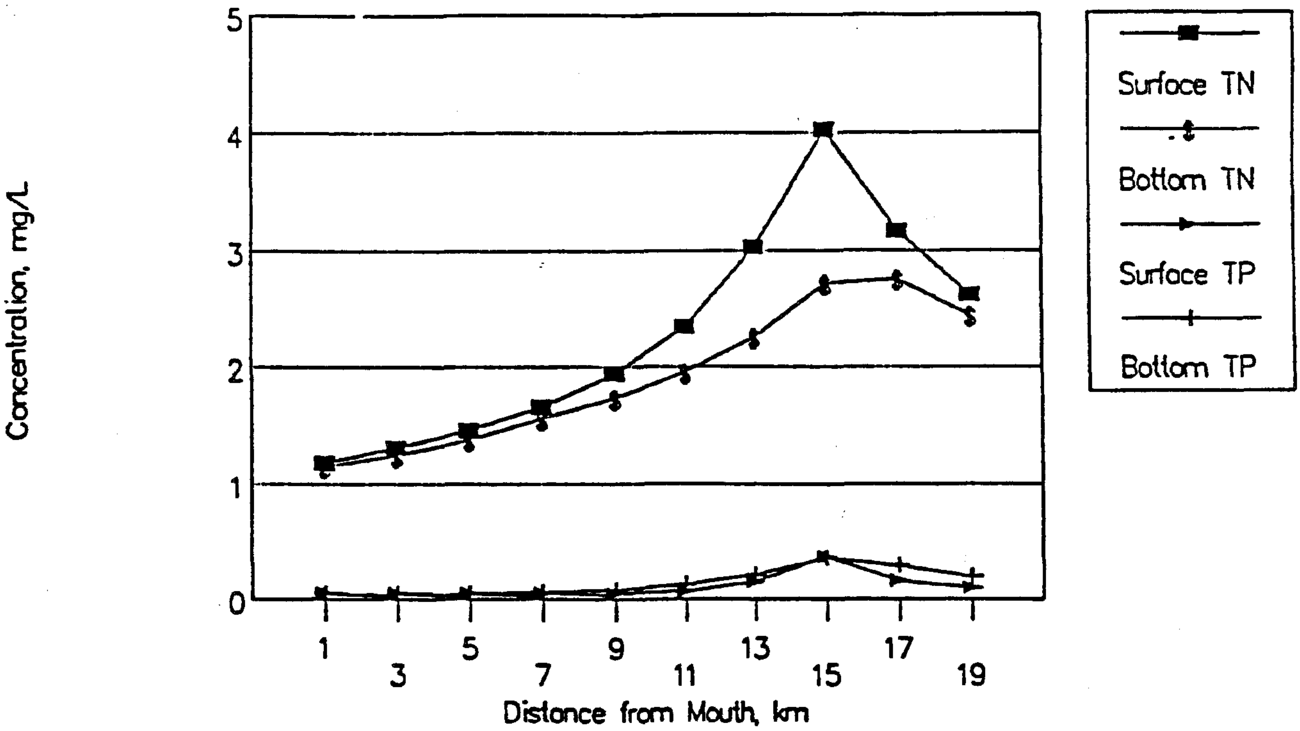

Figure 6-45. Deep Bay total N and P - August 11, surface and bottom.

210 (early November). An extra benthic segment is specified to receive depositing nutrients.

- Dispersion coefficients: Same as salinity simulation.
- Segment volumes: Same as salinity simulation.
- Flows: The same water column flows used in the salinity simulation are used. In addition, settling and deposition velocities for particulate phosphorus are specified.
- Boundary concentrations: Upstream and ocean concentrations of total nitrogen and phosphorus must be specified.
- Pollutant loads: Constant loads of nitrogen and phosphorus in the effluent are specified for the segment adjoining Athens POTW.
- Environmental parameters: No parameters are needed.
- Kinetic constants: No constants are needed.
- Time functions: No time functions are needed.
- Initial conditions: Initial concentrations of total nitrogen and total phosphorus are specified for each segment, along with the dissolved fractions.

Total nitrogen loading from Deep River and Athens POTW were entered and representative settling and deposition velocities of 5 and 2.5 meters/day for particulate phosphorus were input. It was assumed that 80% of the phosphorus and 100% of the nitrogen in the water was dissolved and not subject to settling. Total nitrogen and phosphorus profiles for surface waters during August are shown in Figure 6-45. These profiles indicate nitrogen limitation, as the N:P ratio is less than 25. If all the nitrogen is converted to biomass, then phytoplankton levels of 500 μg/L chlorophyll a are possible near the outfall. Of course light and nutrient limitations to growth along with respiration and death should keep biomass levels to a fraction of this.

Several useful sensitivity studies could suggest possible waste management strategies. First, a component analysis could reveal the relative contributions of Deep River, Athens POTW, and the ocean to total nitrogen and phosphorus throughout Deep Bay. Second, simulations with the effluent at improved secondary and tertiary treatment levels could suggest the expected impact of point source controls. Third, simulations with the river concentrations at various levels could suggest the expected impact of watershed controls.

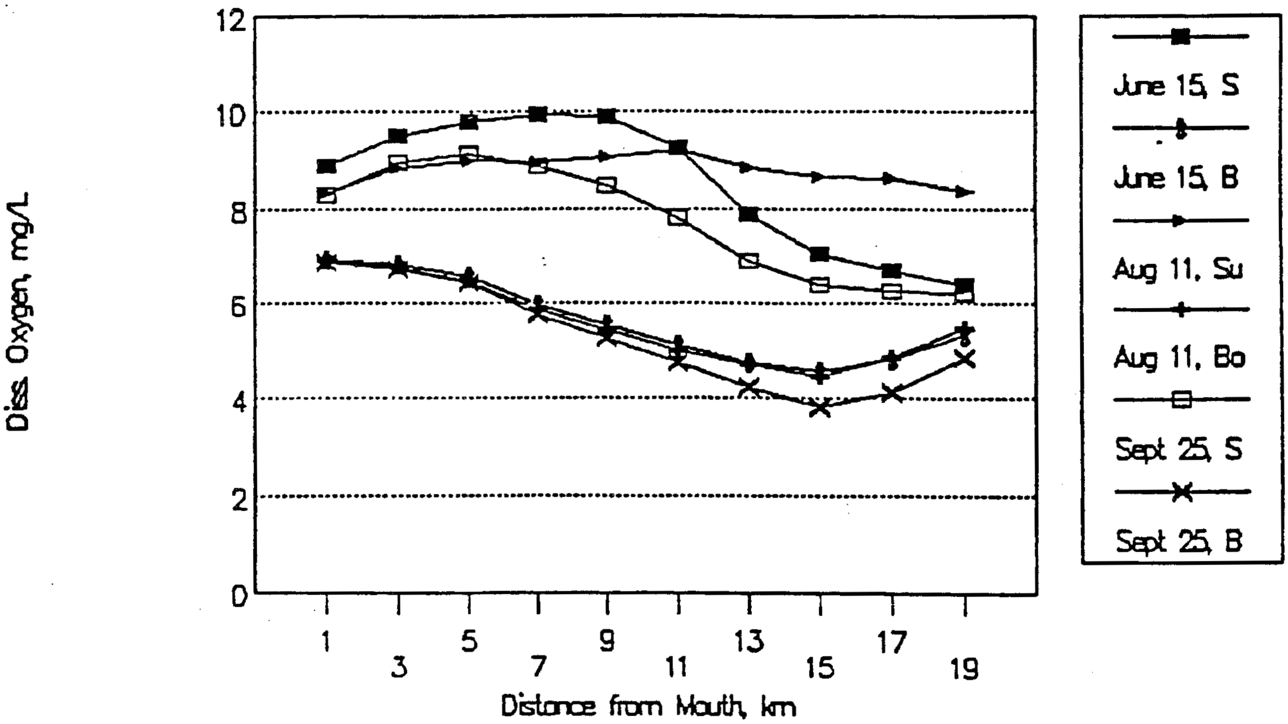

Figure 6-46. Deep Bay dissolved oxygen - June-Sept, surface and bottom.

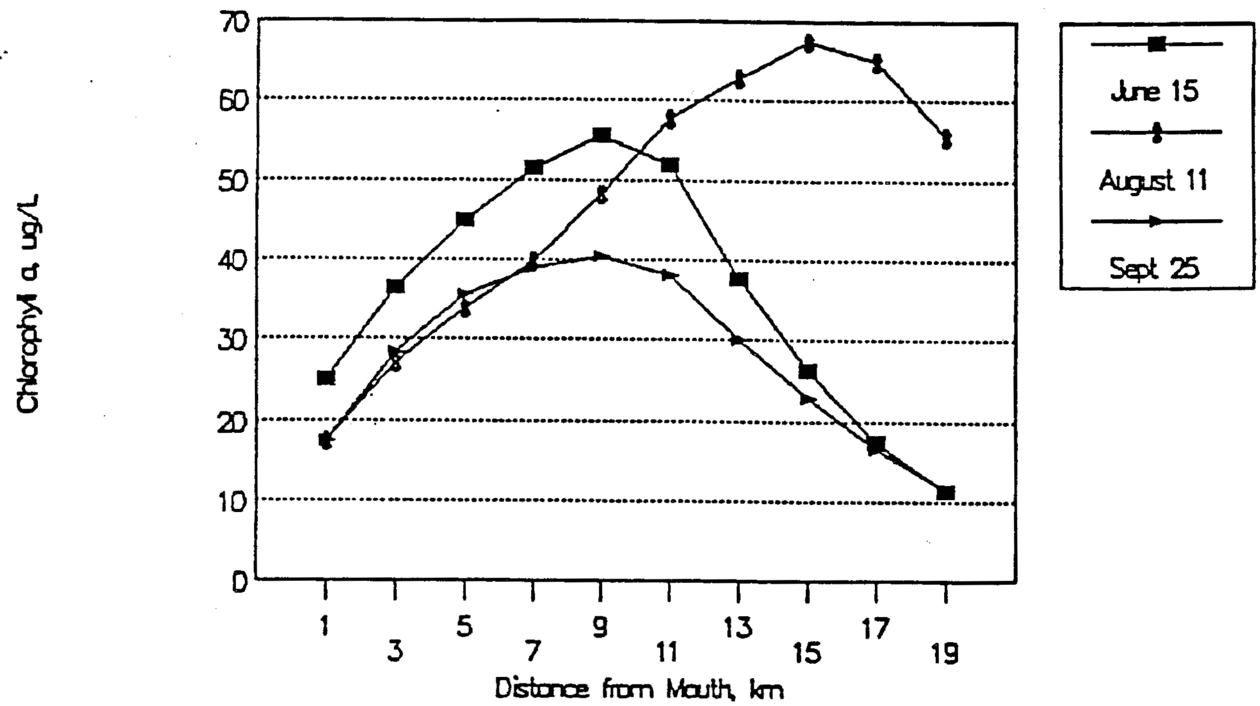

Figure 6-47. Deep Bay phytoplankton - June-Sept, surface.

There are significant advantages and disadvantages in simulating nutrients without phytoplankton to estimate eutrophication potential. The advantages lie in the lessened requirements for field data and modeling resources. Several sites could be evaluated for nutrients only, as compared to the resources required to apply a complex eutrophication model to a single estuary. Further, some states have standards (or goals) for nutrient concentrations and do not require projections of algal density.

The disadvantages of simulating only nutrients relate to several simplifying assumptions required for this type of application. For example, the rate of conversion of dissolved phosphorus into particulate form is dependent upon algal concentration and growth rate. Because algal dynamics are not simulated, these values must be estimated. Further, because algal growth is directly related to nutrient concentrations, calibration parameters may not apply well to future conditions of different nutrient levels. Finally, for situations where algal density is of ultimate concern, nutrient projections alone will only provide an indirect estimate of expected phytoplankton concentrations.

6.4.4 Example 4 - Eutrophication in a Vertically Stratified Estuary

This case study considers simulation of seasonal eutrophication in Deep Bay. The problem setting and model network are as described in the preceding section. Here, the entire eutrophication process is simulated, including nutrients, phytoplankton, carbonaceous BOD, and DO. This is typically the highest level of complexity used for conventional pollution problems. It requires significant amounts of field data and careful calibration to apply with confidence. For this example, it is assumed that two intensive surveys in June and August along with biweekly slack tide surveys allowed calibration of a seasonal simulation. Model information needs are as follows:

- General model information: All 8 systems are used here. Extra benthic segments are specified to simulate long term benthic-water column exchanges of nutrients and DO. The simulation begins on day 1 (April 1), and terminates on day 210 (early November).

- Dispersion coefficients: The same water column dispersion coefficients from the salinity simulation are used. Extra pore water dispersion coefficients for benthic-water column exchange of dissolved chemicals must be specified.

- Segment volumes: The same water column volumes from the salinity simulation are used. A benthic volume underlies each bottom water segment.

- Flows: The same flows from the salinity simulation are used.

- Boundary concentrations: Tributary and ocean concentrations of all 8 systems must be specified.

- Pollutant loads: Constant loads for all 8 systems in the effluent must be specified for the segment adjoining Athens POTW.

- Environmental parameters: Values for average salinity and background sediment oxygen demand for each segment are given. The time variable temperature and light attenuation functions used by each segment must be specified.

- Kinetic constants: Rate constants, temperature coefficients, half saturation constants and other kinetic information must be specified. Processes include nitrification, denitrification, phytoplankton growth (light and nutrient limitation), phytoplankton death, carbonaceous deoxygenation, reaeration, mineralization, and benthic decomposition. If a constant is not specified, then the relevant reaction or process is bypassed.

- Environmental time functions: Time variability in temperature, light extinction, incident light, and length of daylight must be specified.

- Initial conditions: Initial concentrations of each state variable and the fraction dissolved in each model segment are required. The solids settling field affecting each variable must also be specified.

The simulation proceeded from April 1 to November 1, with seasonal light, temperature, and flow data provided. Figures 6-46 and 6-47 show predicted upper layer chlorophyll a and lower level DO during mid July, August and September. Chlorophyll concentrations increase dramatically over the course of the summer, and lower layer DO decreases to a minimum of about 4 mg/L. Diurnal swings about this minimum are predicted to be minimal. The impact of phytoplankton growth is significant on upper layer DO, with levels maintained near saturation and diurnal swings of about one and a half mg/L. Phytoplankton die-off depresses both upper and lower layer DO somewhat. Phytoplankton growth is limited somewhat by nitrogen, but more by light. Sensitivity studies show the relative importance of the variable light attenuation coefficients, the phytoplankton saturating light intensity, and the calibrated Michaelis-Menton nitrogen half saturation coefficient.

Calibration of a model of this complexity is a significant task and cannot be reduced to a neat formula to be summarized here. Some issues of note are the long seasonal or multiyear time scale and the complex interaction among variables, environmental conditions, and kinetic constants. While some water quality models can be calibrated to surveys conducted over a few days, a calibration data set for a eutrophication model typically requires a full season of data. The implications of this are apparent, as data collection programs for model calibration and validation will require years.

Regulations related to eutrophication can differ significantly from state to state. Water quality standards, criteria, or goals can relate to chlorophyll, transparency, nutrients, and/or DO. Selection of critical conditions is very difficult because of the need to characterize a season or even an entire year, not a single day or event. This is complicated by the kinetic interactions. For example, light attenuation is often critical, but choice of reasonable design extinction coefficients is not often given sufficient study. Actual data for a representative or drought year are often used instead of statistical characterizations of design conditions. As another approach, constant steady conditions of statistical significance are also used.

For performing a waste load allocation on Deep Bay, the calibration year combining high spring flows with very low summer flows and warm temperatures was judged to provide reasonable worst case conditions. A series of simulations with various combinations of POTW treatment levels and watershed controls were performed. It was concluded that tertiary treatment without watershed controls could still result in phytoplankton levels of 30 μg/L and lower DO levels of 4.5 mg/L. A combination of watershed controls and advanced secondary treatment was judged most reasonable.

6.4.5. *Example 5 - Ammonia Toxicity in a Two-Dimensional Estuary*

The fifth and sixth examples consider toxic pollutants in a laterally variant two-dimensional estuary. This type of estuary characterization differs from the previous two in that lateral variations in water quality are significant enough that the estuary cannot be assumed to be laterally well mixed. The need for describing lateral variation in water quality sometimes is dictated by the pollutant of concern as well as the nature of the system. For example, point sources of pollutants that act in an indirect manner (e.g. oxygen demanding substances, algal nutrients) often can be treated as laterally homogeneous even when significant lateral gradients exist near the outfall. These pollutants typically exert their maximum influence a significant distance away from the outfall, where conditions are more likely to be laterally well mixed. Direct-acting pollutants such as those causing acute toxicity will often require lateral variation to be described, as concentrations near the outfall (where lateral gradients will be highest) are of primary concern.

For model application to a two-dimensional estuary, multiple segments extend across the width of the estuary, allowing for the description of lateral changes in water quality. Depending upon the degree of vertical stratification, the system can be treated as two-dimensional (no vertical stratification) or three-dimensional (with vertical stratification). Again, vertical layer(s) to describe sediment quality can be added to either framework (using WASP4) when necessary to describe sediment/water interactions.

The fifth case study concerns ammonia toxicity and is simulated using the kinetic submodel TOXI4. Ammonia toxicity is often a concern near discharges of municipal waste, as the unionized form of ammonia is toxic to fish and other aquatic life. Two processes are simulated - the dissociation of ammonia to ionized and aqueous forms and the first-order loss of total ammonia through nitrification. Model kinetic inputs for this simulation are quite straightforward. All that is required is a description of the ionization constant for ammonia and the ammonia loss rate.

6.4.5.1. Problem Setting

The City of Boatwona, population 285,000, is located on the shore of the Boatwona Bay (Figure 6-48). This relatively shallow estuary is driven by moderate 0.50 meter tides and a medium but seasonably variable inflow from the Boatwona River, which is gauged above the fall line. The Boatwona estuary provides for a rich commercial fishing and shellfishing industry. Boating and recreational fishing are popular, as are several bathing beaches.

Just outside the City of Boatwona is a large fertilizer plant which discharges into the estuary. Because this discharge is high in ammonia there have been instances of ammonia toxicity in the bay. Unionized ammonia is toxic to fish at fairly low concentrations. The water quality criterion is 0.08 mg/L for a 30 day average.

Bathymetric surveys have produced a chart of soundings at low tide, used for navigation (Figure 6-49). Three surveys were conducted (May, August and November) to characterize tide, temperature, and pH. Continuous velocity data, temperature data and pH data were obtained from moorings at sampling stations S1, S2, and S3 over these three five-day periods (Table 6-15).

The Boatwona River flow, Ammonia and pH data are summarized as monthly averages (Table 6-16).

6.4.5.2. Boatwona Estuary Network

Analysis of the monitoring data illustrates a definite lateral flow pattern. Because of these lateral flows, the bay was segmented to demonstrate the fate and transport of the ammonia discharge (Figure 6-50). Segments were defined every 5 kilometers, giving 6 water column segments.

6.4.5.3. Boatwona Estuary Nitrogen Simulation

The WASP4 model was given flow information averaged from the continuous flow meters that were installed during the sampling surveys:

- General model information: One system is simulated - system 1 is interpreted as total ammonia-nitrogen. The organic toxic chemical model TOXI4 was used for this study because of its capabilities of simulating both unionized and ionized forms of chemicals. The remaining sys-

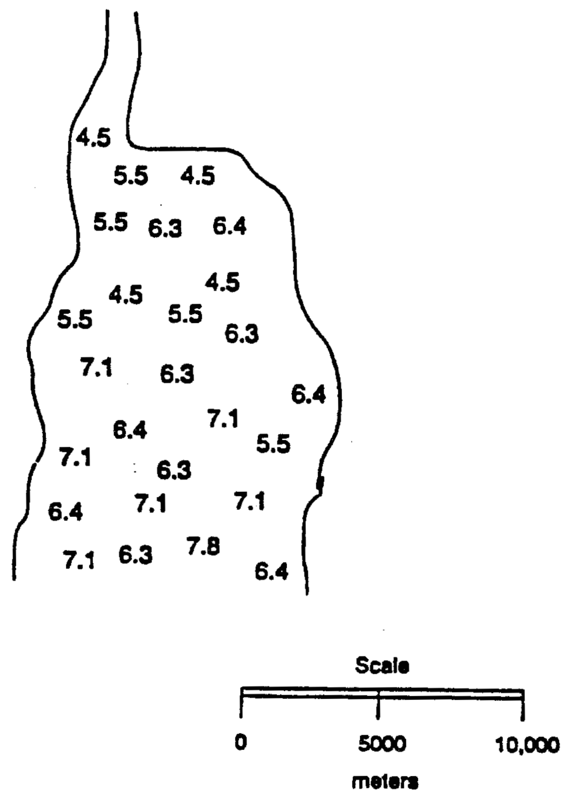

Figure 6-49. Boatwona Estuary depth chart.

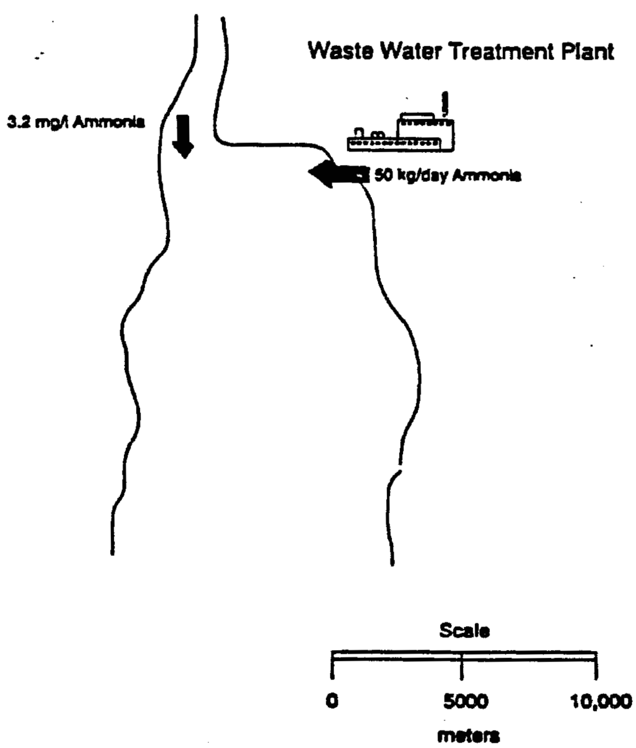

Figure 6-48. City of Boatwona waste water treatment plant location.

Table 6-15. Boatwona Estuary Survey Data

	S1		S2		S3	
Sample Time	Temp	pH	Temp	pH	Temp	pH
May	17.0	6.8	16.5	7.1	15.3	6.9
August	19.2	6.9	18.2	6.9	17.0	7.0
Nov	17.4	6.8	16.7	6.8	16.9	6.8

Table 6-16. Boatwona River Survey Data

Month	Average Flow (cms)	pH	N
January	12	6.2	2.3
February	15	6.4	0.8
March	18	6.1	2.1
April	22	6.2	4.2
May	15	6.6	6.6
June	11	6.8	2.3
July	8	6.9	9.4
August	10	7.1	7.3
September	15	6.8	3.7
October	13	6.8	0.9
November	14	6.6	1.3
December	13	6.7	4.2

tems are bypassed. The simulation begins on day 21, representing the April 21 survey, and ends on day 147, a week following the August 11 survey.

- Dispersion coefficients: This estuary requires longitudinal dispersion coefficients. We can neglect the vertical diffusion as the estuary exhibited no vertical stratification. The dispersion terms were used to simulated the effects of tidal mixing.
- Segment volumes: Mean tide volumes are specified for all segments.
- Flows: Tributary flow is routed into the estuary. Mean monthly river flows are specified.
- Boundary concentrations: Monthly averaged ammonia concentrations are assumed for the Boatwona River. The seaward boundaries are assumed zero.
- Pollutant loads: Based upon continuous monitoring studies conducted at the fertilizer plant.
- Model parameters: Specification of temperature and pH distribution both spatially and temporally.
- Kinetic constants: Ionization constants and nitrification rate for ammonia.
- Environmental time functions: Temporal temperature functions.
- Initial concentrations: Initial ammonia concentrations within the estuary are assumed zero. Dissolved fractions are set to 1.0.

Figure 6-51 shows selected output from this simulation of ionized/un-ionized ammonia concentrations over time in the segment receiving the loading. Model calibration would consist of conducting a dye study as previously mentioned. A dye study would then be followed by calibration of the ammonia loss rate to total ammonia data. Ammonia dissociation parameters are chemical constants and do not require adjustment during the calibration process.

It is important to note that the ammonia loss rate is a lumped parameter, combining (potentially) several different processes. The dominant loss process will typically be nitrification, but also will include phytoplankton uptake. Hydrolysis of organic nitrogen and sediment ammonia release can also affect the net loss rate. Algal

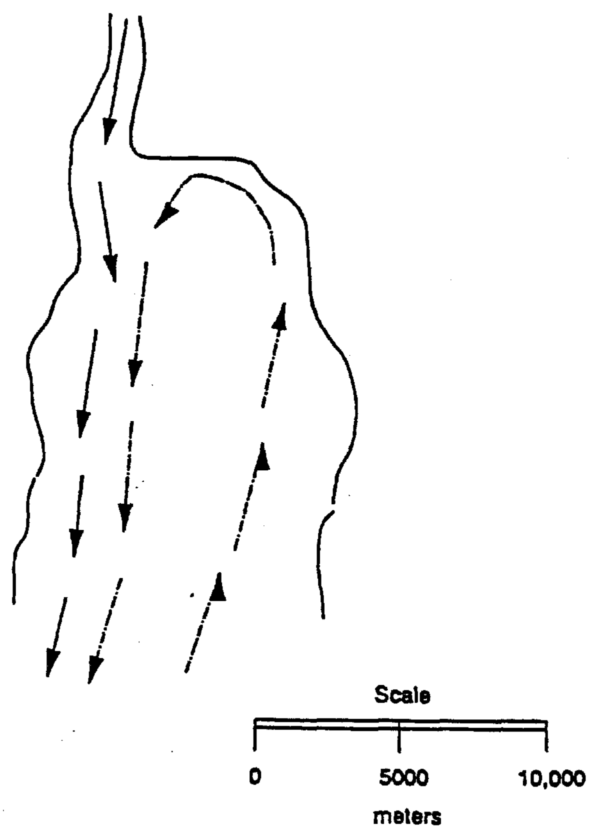

Figure 6-50. Boatwona Estuary flow pattern.

uptake/recycle of ammonia can be especially important in eutrophic systems.

Waste load allocation for ammonia toxicity consists of determining the maximum allowable loading to comply with water quality standards at critical environmental conditions. pH must be included with temperature and flow as an important environmental condition, as pH and temperature determine the percentage of total ammonia in un-ionized form. It should be noted that there is uncertainty in the appropriateness of current ammonia criteria, due to the limited range of data available in describing toxicity. Current research indicates that the toxicity of the un-ionized ammonia may vary with changes in temperature and pH. This information is not reflected in present criteria.

6.4.6. *Example 6: Alachlor in a Laterally Variant Estuary*

The sixth example study considers the fate of a hydrophilic, reactive chemical in a two- dimensional estuary. This example represents simulation of any hydrophilic, reactive chemical. These chemicals typically have relatively high solubility and low affinity for solids, and are subject to transformation (and possible degradation) in the environment. Possible transformation processes include hydrolysis, photolysis, oxida-

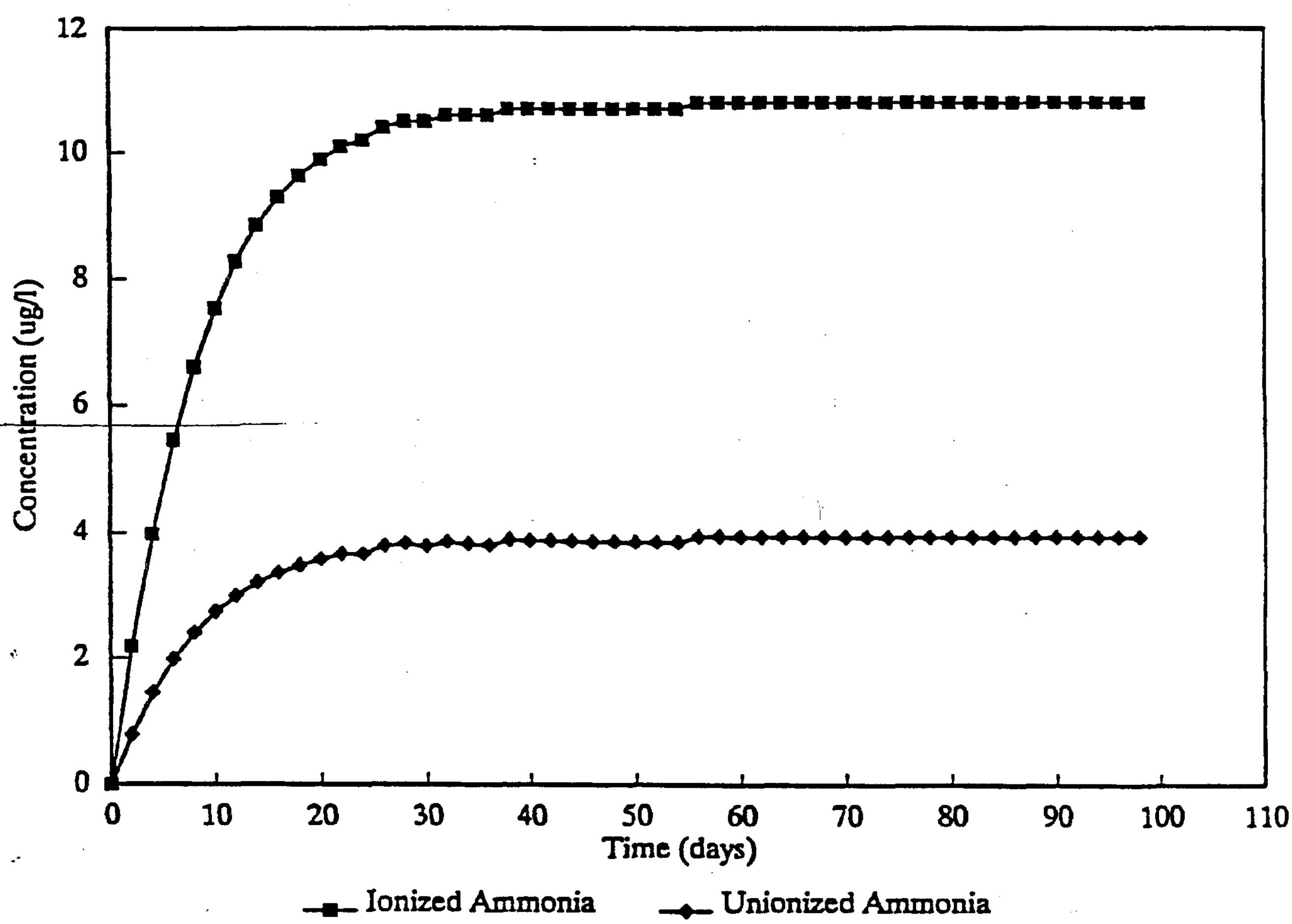

Figure 6-51. Ammonia simulation results.

tion, reduction, and biodegradation. In addition, volatilization can lead to loss of chemical from the water.

The same estuary is used as for example 5; however, benthic sediments also are being considered. Two layers of benthic sediments are simulated - upper surficial sediment and deep sediments. This simulation uses Systems 1 through 3 in TOXI4. Two types of solids are represented, corresponding to inorganic and organic materials, respectively. System 1 represents the pollutant. System 2 represents inorganic solids, and System 3 represents organic solids. Environmental fate parameters for this simulation are those for the pesticide Alachlor, and were taken from Schnoor et al. (1987). Volatilization and hydrolysis were found to be insignificant for this pollutant, with biodegradation serving as the main route of degradation. Biodegradation will be treated as a first-order loss process for this simulation, with separate values used for the water column and the sediment.

Readers viewing the input file will find that it varies only slightly from the one for the previous example. Ionization coefficients have been removed. The first-order biodegradation rate constants are lower, and the partition coefficient is higher than values in the previous example. Figure 6-52 displays selected results for the input values, indicating the response of the water column and benthic sediments to changes in pollutant loading. No discussion of the WLA significance of this example is given. This example is provided primarily to serve as a template for general application.

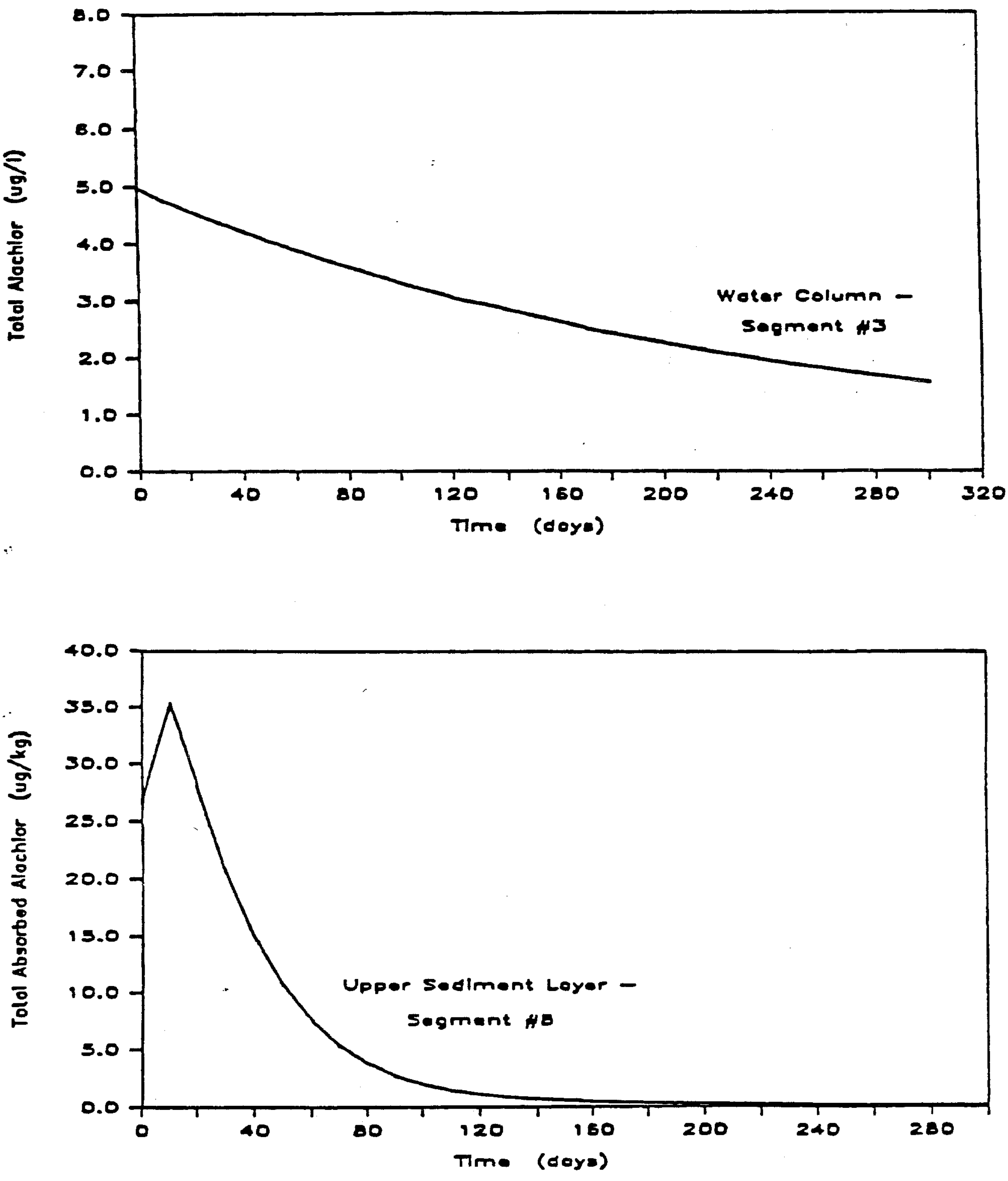

Figure 6-52. Hydrophobic (Alachlor) chemical simulation for example 6.

6.5 References

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