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SELECTING ESTUARINE MODELS

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SECTION I

INTRODUCTION

I.1 PURPOSE

This chapter on selection of estuarine models is one in a series of manuals whose purpose is to provide technical information and policy guidance for the preparation of Waste Load Allocations (WLAs). The objective of such waste load allocations is to ensure that water quality conditions are achieved that protect the designated beneficial uses of the receiving water. An ancillary benefit of a technically sound WLA is that excessive degrees of treatment which are not necessary and that do not yield proportionate improvements in water quality, can be avoided.

I.2 RELATION TO OTHER BOOKS AND CHAPTERS

The various books and chapters that make up the set of technical guidance manuals on Waste Load Allocation are summarized in Chapter 1-1. These technical chapters should be used in conjunction with the material of Book I which provides background information applicable to all types of water bodies and to all contaminants that must be considered in the Waste Load Allocation process.

I.3 SCOPE OF CHAPTER

I.3.1 IMPORTANCE OF NUTRIENTS AND TOXICS IN THE ESTUARY

The most significant anthropogenic impacts on estuaries stem from the release of nutrients and toxic chemicals to feeder streams and to the estuary itself. Nutrients appear to present the greatest threat to the estuary because of their role in supporting and promoting the widespread growth of algae. Algal growths are important because they act to diminish the penetration of sunlight into the water. Submerged aquatic vegetation

TABLE I-1

ORGANIZATION OF GUIDANCE MANUAL FOR PERFORMANCE OF WASTE LOAD ALLOCATIONS

BOOK I	GENERAL GUIDANCE (Discussion of overall WLA process, procedures and considerations)	
BOOK II	STREAMS AND RIVERS (Specific technical guidance for these water bodies)	
	Chapter 1	BOD/Dissolved Oxygen Impacts and Ammonia Toxicity
	2	Nutrient/Eutrophication Impacts
	3	Toxic Substances Impacts
BOOK III	ESTUARIES	
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BOOK IV	LAKES, RESERVOIRS, AND IMPOUNDMENTS	
	Chapter 1	BOD/Dissolved Oxygen Impacts
	2	Nutrient/Eutrophication Impacts
	3	Toxic Substances Impacts

Note: Other water bodies (e.g., groundwaters, bays, and oceans) and other contaminants (coliform bacteria and virus, TDS) may subsequently be incorporated into the manual as need for comprehensive treatment is determined.

(SAV) is dependent upon sunlight for photosynthesis, and when light penetration is diminished too much by algal growths, the SAV will be affected.

SAV serves an important role as habitat and food source for much of the biota of the estuary. Major estuary studies, including an intensive years-long study of the Chesapeake Bay, have shown that the health of SAV communities serves as an important indication of estuary health. When SAV communities are adversely affected by nutrients and/or toxics, the aquatic life use of the estuary will also be affected.

I.3.2 BENEFICIAL USES IN THE ESTUARY

Our national management strategy for surface waters is based upon the specification, by each State, of a water quality standard for individual water bodies or portions of a water body within that State. Once specified, the standard becomes the gage against which general water quality is assessed for the specified water body.

A standard is made up of two components: an aquatic life protection use, and water quality criteria that will protect that use. The starting point in the specification of a standard is the definition of attainable uses for the water body in question. The basic precepts for the specification of uses in an estuary are discussed in two documents issued by the U.S. Environmental Protection Agency, Office of Water Regulations and Standards: Water Quality Standards Handbook (December, 1983) and Technical Support Manual: Water Body Surveys and Assessments for Conducting Use Attainability Analyses, Volume II, Estuaries (June, 1984).

'Cold water fishers,' 'warm water fishers,' or 'fish maintenance' are examples of aquatic life protection uses. The use most commonly found in State standards that is applicable to the estuary is generally phrased in terms of the protection and propagation of fish and shellfish. For the simple estuary with few freshwater sources, the delineation of a zone whose salinity range will support the protection and propagation of fish and shellfish may be straightforward. For the larger, more complex estuary, however, the physiography of individual embayments, and the presence of regionalized water chemistry-water quality characteristics may require greater specificity in the establishment of uses. Uses are protected by criteria, the levels of various water quality constituents that will support (in the case of dissolved oxygen) or not interfere (in the case of pH, temperature, ammonia, chlorine, cadmium, etc.) with the normal life processes of the aquatic life forms of the estuary.

Waste Load Allocation (WLA) studies are conducted in order to assure that the cumulative waste discharges to a water body will not violate standards or jeopardize the uses that are to be maintained by adherence to the standard. The complexity of a waste load allocation study will vary with the complexity of the water body to be examined and the number of discharges to the water body. Complexity in the estuary is manifested by many factors--tidal, wind, and Coriolis forces that establish circulation patterns; temperature and salinity gradients that cause stratification; nutrients, toxics, and oxygen demanding wastes that shape water quality and directly affect aquatic plants and animals--that may necessitate a highly sophisticated approach to waste load allocation studies.

Estuarine waste load allocation studies generally require the use of a mathematical model in order to understand the ultimate disposition of wastes. A wide variety of models have been developed to address the spectrum of complexity that may be encountered in estuaries. The models may range in sophistication from those that are readily run with a hand held calculator to those that require the most powerful computers; from those that consider a waste to be conservative to those that consider the kinetic and thermodynamic properties of toxic wastes; and from those that consider a waste to be completely mixed upon introduction to the water body to those that consider the transport of a waste in three dimensions, as controlled by circulation and stratification.

I.3.3 OBJECTIVES OF CHAPTER

The objective of this Chapter is to provide the reader with explicit guidance in the selection of a model that best satisfies the requirements of a specific waste load allocation study, and that best represents the conditions in the estuary of concern.

I.4 OVERVIEW OF CRITERIA FOR SELECTION OF A MODEL

There are numerous publications that competently describe the characteristics and capabilities of individual models that may be used in an estuarine study, and other publications that compare the attributes of these models, one with another, but little indeed in the literature that provides systematic guidelines for the selection of an appropriate model.

The appropriateness of a model is determined by examining the estuary in terms of spatial and temporal characteristics in order to decide whether a zero, one, two or three dimensional analysis is required; to decide the time scale of the analysis and which temporal processes (the most important of which is tide in a short scale, or seasonal freshwater flows on a longer scale, etc.) are important.

SECTION II

HYDRODYNAMIC AND MASS TRANSPORT PROCESSES

II.1 GENERAL

The term estuary is generally used to denote the lower reaches of a river where tide and river flows interact. The generally accepted definition for an estuary was provided by Pritchard in 1952: "An estuary is a semi-enclosed coastal body of water having a free connection with the open sea and containing a measureable quantity of seawater." This description has remained remarkably consistent with time and has undergone only minor revisions (Emery and Stevenson, 1957; Cameron and Pritchard, 1963). To this day, such qualitative definitions are the most typical basis for determining what does and what does not constitute an estuary.

Estuaries are perhaps the most important social, economic, and ecologic regions in the United States. For example, according to the Department of Commerce (DeFalco, 1967), 43 of the 110 Standard Metropolitan Statistical Areas are on estuaries. Furthermore, recent studies indicate that many estuaries, including Delaware Bay and Chesapeake Bay, are on the decline. Thus, the need has arisen to better understand their ecological functions to define what constitutes a "healthy" system, to define actual and potential uses, to determine whether designated uses are impaired, and to determine how these uses can be preserved or maintained.

As part of such a program, there is a need to define impact assessment procedures that are simple, in light of the wide variability among estuaries, yet adequately represent the major features of each system studied. Estuaries are three-dimensional waterbodies which exhibit variations in physical and chemical processes in all three directions (longitudinal, vertical, and lateral) and also over time. However, following a careful consideration of the major physical and chemical processes and the time scales involved in a particular study one can often define a simplified version of the prototype system for study.

In this chapter, a discussion is presented of the important estuarine features and major physical processes. From this background, guidance for model selection is given which considers the various assumptions that may be made to simplify the complexity of the analysis, while retaining an adequate description of the system. Finally, a framework for selecting appropriate computer models is outlined in Chapter IV.

II.2 PHYSICAL PROCESSES

II.2.1 INTRODUCTION

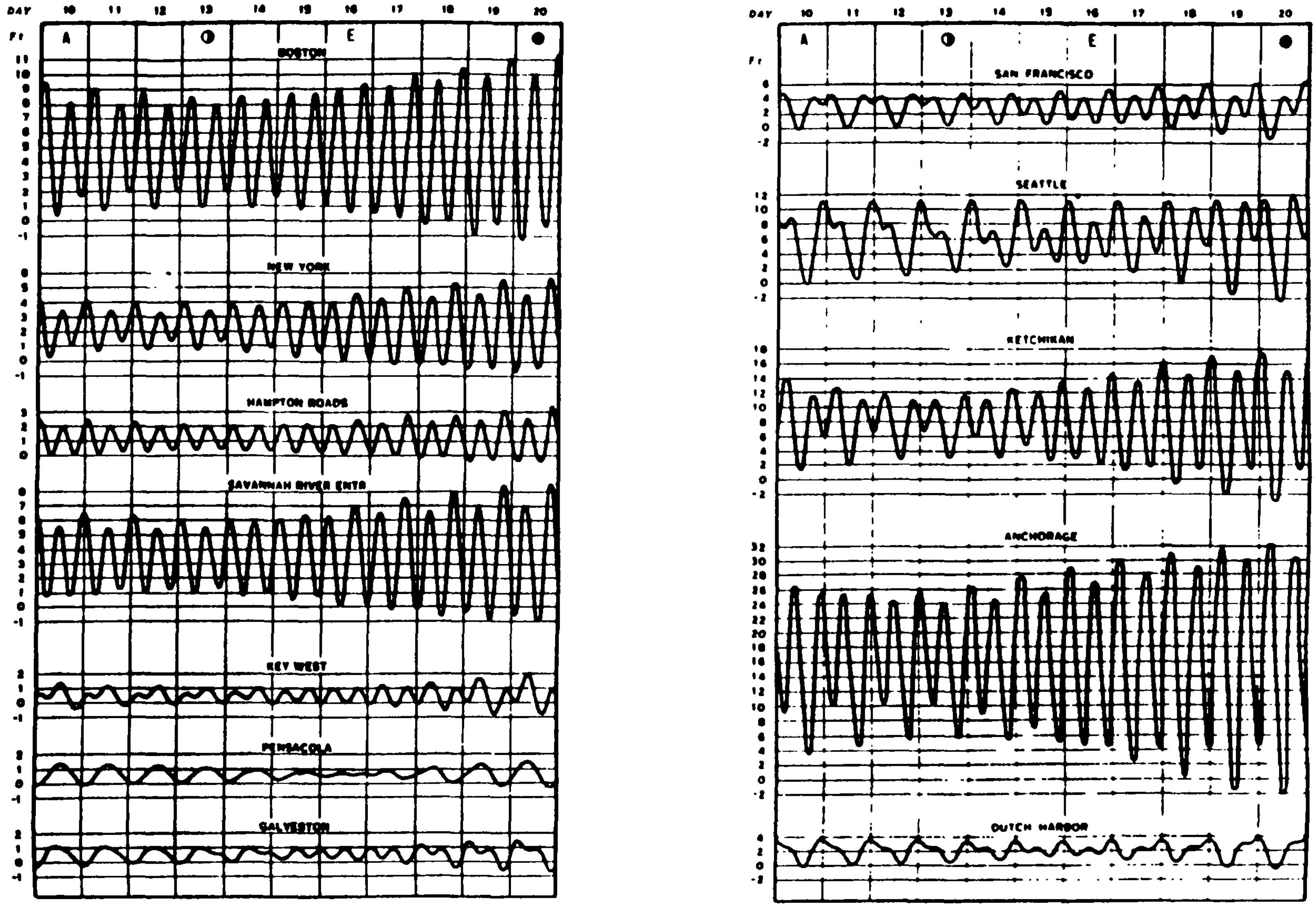
Estuarine flows are the result of a complex interaction of:

- o tides,
- o wind,
- o freshwater inflow,
- o bottom friction,
- o Rotational effect of the earth (Coriolis effect),
- o vertical mixing, and
- o horizontal mixing.

In performing a modeling study, one tries to simplify the complex prototype system by determining which of these effects or combination of effects is most important at the time scale of the evaluation. To do this, it is necessary to understand each of these processes and their impacts on the evaluation. A complete description of all of the above is beyond the scope of this chapter. Rather, illustrations are provided of some of the features of each process, which emphasize considerations of magnitude and time scale.

II.2.2 TIDES

Tides are highly variable throughout the United States, both in amplitude and phase. Figure II-1 (NOAA, 1983) shows some typical tide curves along the Atlantic, Gulf of Mexico, and Pacific Coasts. Tidal amplitude can vary from 1 foot or less along the Gulf of Mexico (e.g., Pensacola, Florida) to



A discussion of these curves is given on the preceding page.

Lunar data: A - Moon in apogee
◐ - last quarter
E - Moon on Equator
● - new Moon

A discussion of these curves is given on the preceding page.

Lunar data: A - Moon in apogee
◐ - last quarter
E - Moon on Equator
● - new Moon

Figure II-1. Typical Tide Curves for United States Ports.

over 30 feet in parts of Alaska (e.g., Anchorage) and the Maritime Provinces of Canada (e.g., the Bay of Fundy). Tidal phasing is a combination of many factors with differing periods. However, in the United States, most tides are based on 12.5-hour (semidiurnal), 25-hour (diurnal) and 14-day (semi-lunar) combinations. In some areas, such as Boston (Figure II-1), the tide is predominantly semidiurnal with 2 high tides and 2 low tides each day. In others, such as along the Gulf of Mexico, the tides are more typically mixed.

Tidal power is directly related to amplitude. This potential energy source can promote increased mixing through increased velocities and interactions with topographic features.

II.2.3 WIND

In many exposed bays or estuaries, particularly those in which tidal forcing is smaller, wind shear can have a tremendous impact on circulation patterns at time scales of a few hours to several days. An example is Tampa Bay on the West Coast of Florida, where tidal ranges are approximately 3 feet, and the terrain is generally quite flat. Wind can be produced from localized thunderstorms of a few hours duration, or from frontal movements with durations on the order of days. Unlike tides, wind is unpredictable in a real time sense. The usual approach to studying wind driven circulation is to develop a wind rose (Figure II-2) from local meteorological data, and base the study of impacts on statistically significant magnitudes and directions, or on winds that might produce the most severe impact.

II.2.4 FRESHWATER INFLOWS

Freshwater inflows from a major riverine source can be highly variable from day to day and season to season. At the shorter time scale, the river may be responding to a localized thunderstorm, or the passage of a front. In many areas, however, the frequency of these events tends to group into a season (denoted the wet season) which is distinct from the remainder of the year (the dry season). The average monthly streamflow distributions in

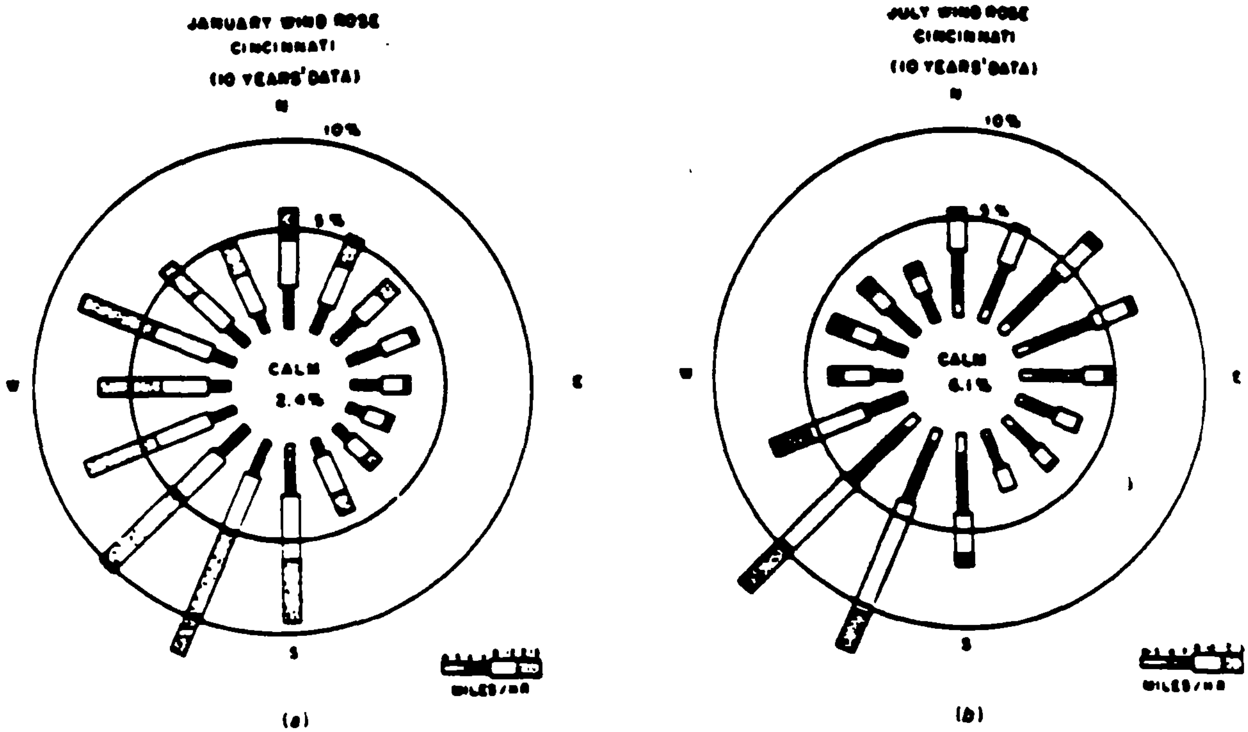


Figure II-2. Typical Wind Rose. (H.C. Perkins, 1974)

Figure II-3 illustrate that in Virginia the wet season is typically from December to May and comes mainly from frontal systems. In Florida, however, where the wet season coincides with the summer months when localized thunderstorms predominate, the trend is reversed.

It is important to consider the effect of freshwater flows on estuarine circulation because streamflow is the only major mechanism which produces a net cross-sectional flow over long averaging times. A common approach is to represent the estuary as a system driven by net freshwater flows in the downstream direction with other effects averaged out and lumped into a dispersion-type parameter. When using this approach to evaluate the estuary system, one must weigh the consequences very carefully.

Freshwater is less dense and tends to "float" over seawater. In some cases, freshwater may produce a residual 2-layer flow pattern (such as in the James Estuary, Virginia, or Potomac River) or even a 3-layer flow pattern (as in Baltimore Harbor). The danger is to treat such a distinctly 2-layer system as a cross-sectionally averaged, river driven system, and then try to explain why pollutants are observed upstream of a discharge point when no advective mechanism exists to produce this effect using a one-dimensional approach.

II.2.5 FRICTION

The estuary's topographic boundaries (bed and sides) produce frictional resistance to local currents. In some estuaries with highly variable geometries, this can produce a number of net nontidal (or tidally-averaged) effects such as residual eddies near headlands or tidal rectification. Pollutants trapped in residual eddies, perhaps from a wastewater treatment plant outfall, may have very large residence times that are not predictable from cross-sectionally averaged flows before such pollutants are flushed from the system.

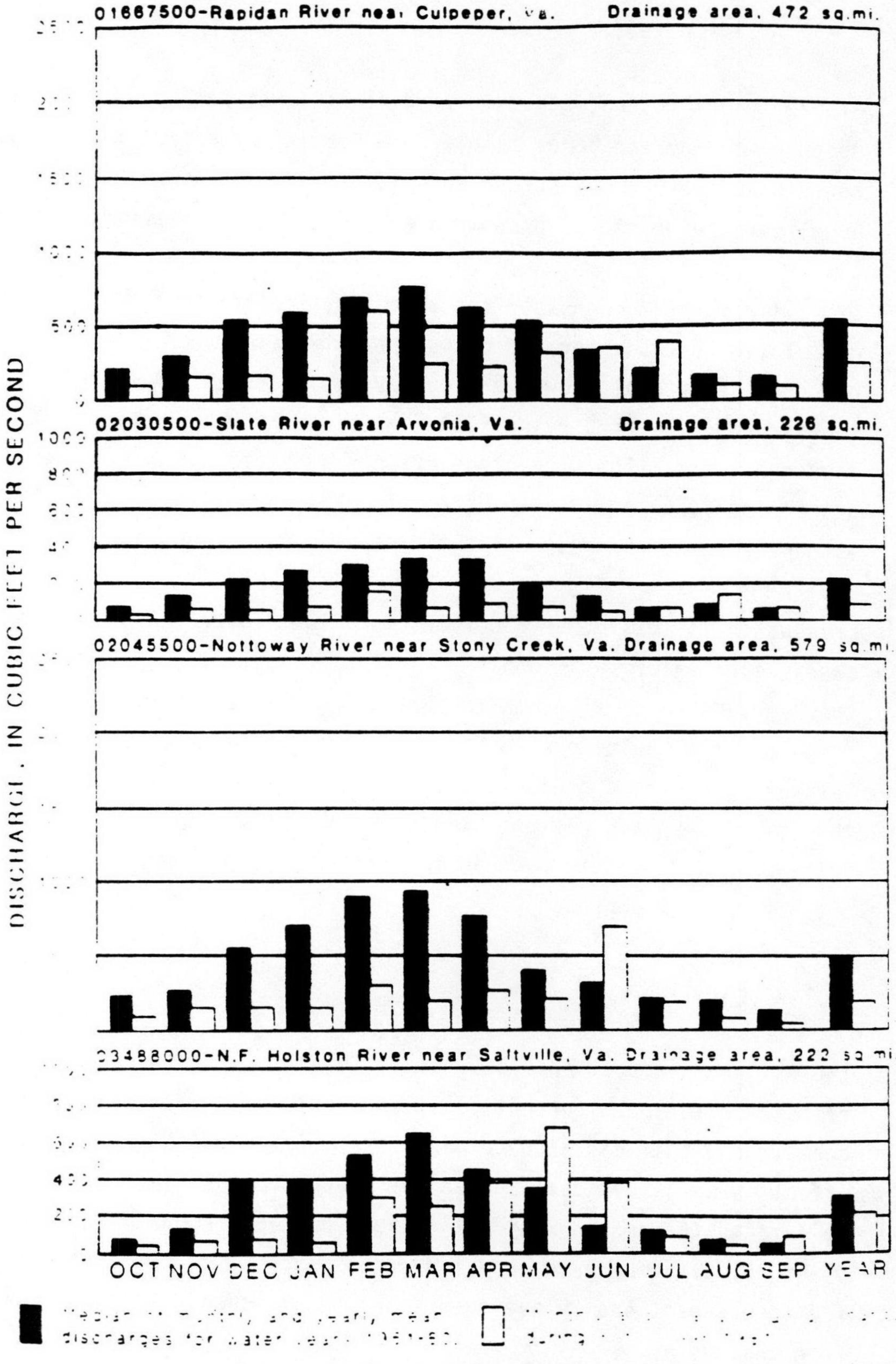


Figure II-3. Monthly Average Streamflows for Locations in Virginia. (from U. S. Geological Survey 1982)

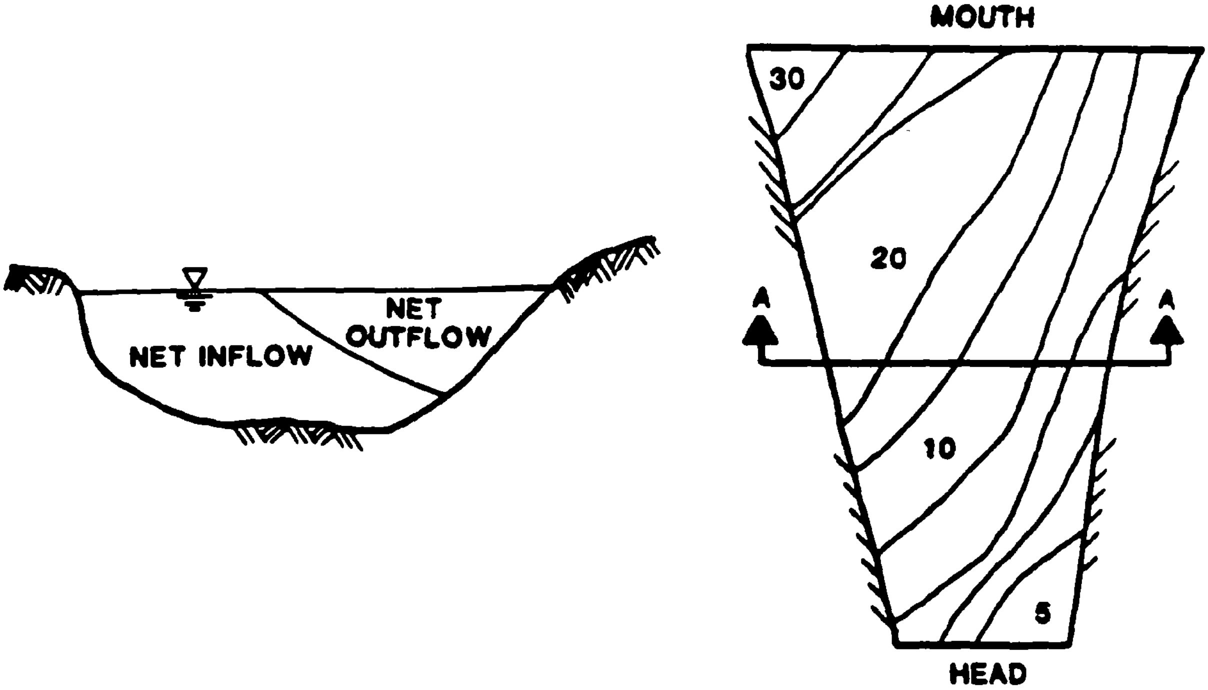
II.2.6 CORIOLIS EFFECT

In wide estuaries, the Coriolis effect can cause freshwater to move to the right-hand bank (facing the open sea) so that the surface slopes upward to the right of the flow. The interface has an opposite slope to maintain geostrophic balance. For specific configurations and corresponding flow regimes, the boundary between outflow and inflow may actually cut the surface (Figure II-4a). This is the case in the lower reaches of the St. Lawrence estuary, for example, where the well-defined Gaspe Current holds against the southern shore and counter flow is observed along the northern side. This effect is augmented by tidal circulation which forces ocean waters entering the estuary with the flood tide to adhere to the left side of the estuary (facing the open sea), and the ebb flow to the right side. Thus, as is often apparent from the surface salinity pattern in an estuary, the outflow is stronger on the right-hand side (Figure II-4b). The exact location and configuration of the saltwater/freshwater interface depends on the relative magnitude of the forces at play. Quantitative estimates of various mixing modes in estuaries are discussed below.

II.2.7 VERTICAL MIXING

All mixing processes are caused by local differences in velocities and by the fact that liquids are viscous (i.e., possess internal friction). In the vertical direction, the most common mixing occurs between riverine fresh waters and the underlying saline ocean waters.

If there were no friction, freshwater would flow seaward as a shallow layer on top of the seawater. The layer would become shallower and the velocity would decrease as the estuary widened toward its mouth. However, the fact of friction between the two types of water requires a balancing pressure gradient down-estuary, explaining the salt wedge formation which deepens toward the mouth of the estuary, as seen in Figure II-5. Friction also causes mixing along the interface. A particularly well-defined salt wedge is observed in the estuary of the Mississippi River.



a. Cross-section A-A looking Down-estuary.

b. Surface Salinity Distribution (ppt).

Figure II-4. Net Inflow and Outflow in a Tidal Estuary, Northern Hemisphere.

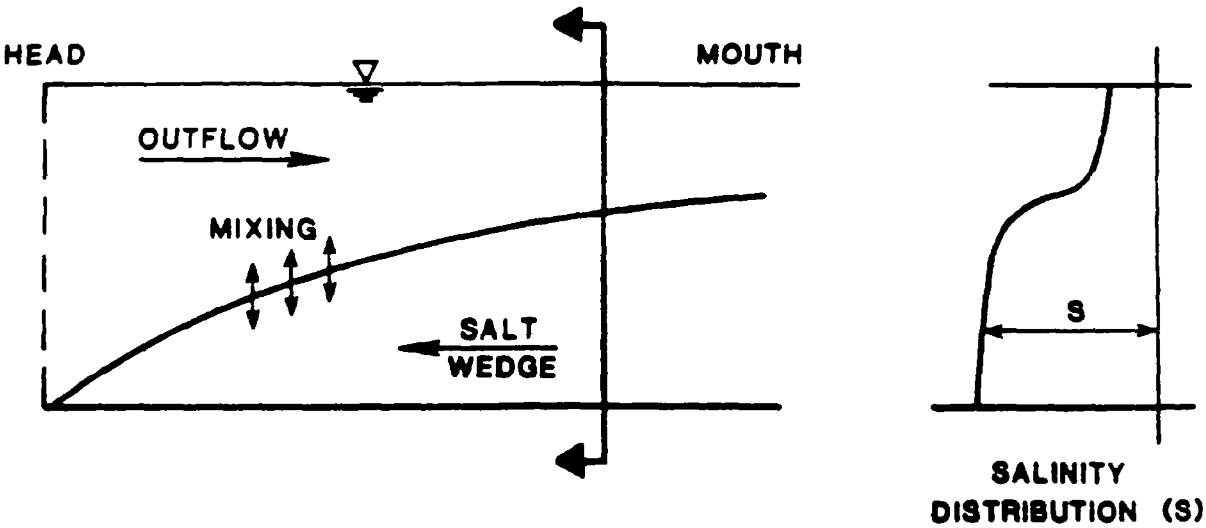


Figure II-5. Layered Flow in a Salt-wedge Estuary (Longitudinal Profile).

If significant mixing does not occur along the freshwater/saltwater interface, the layers of differing density tend to remain distinct and the system is said to be highly stratified in the vertical direction. If the vertical mixing is relatively high, the mixing process can almost completely break down the density difference, and the system is called well-mixed or homogeneous.

In sections of the estuary where there is a significant difference between surface and bottom salinity levels over some specified depth (e.g., differences of about 5 ppt or greater over about a 10 foot depth), the water column is regarded as highly stratified. An important impact of vertical stratification is that the vertical density differences significantly reduce the exchange of dissolved oxygen and other constituents between surface and bottom waters. Consequently, persistent stratification can result in a depression of dissolved oxygen (DO) in the high salinity bottom waters that are cut off from the low salinity surface waters. This is because bottom waters depend upon vertical mixing with surface waters, which can take advantage of reaeration at the air-water interface, to replenish DO that is consumed as a result of respiration and the decay of organic materials within the water column and bottom sediments. In sections of the estuary exhibiting significant vertical stratification, vertical mixing of DO contributed by reaeration is limited to the low salinity surface waters. As a result, persistent stratified conditions can cause the DO concentration in the bottom waters to fall to levels that cause stress on or mortality of the resident communities of benthic organisms.

Another potential impact of vertical stratification is that anaerobic conditions in bottom waters can result in increased release of nutrients such as phosphorus and ammonia-nitrogen from bottom sediments. During later periods or in sections of the estuary exhibiting reduced levels of stratification, these increased bottom sediment contributions of nutrients can eventually be transported to the surface water layer. These increased nutrient loadings on surface waters can result in higher phytoplankton concentrations that can exert diurnal DO stresses and reduced light penetration for rooted aquatic plants. In summary, the persistence and areal extent of vertical stratification is an important determinant of mixing within an estuary.

II.2.8 HORIZONTAL MIXING

Mixing also occurs in the horizontal direction, although it is often neglected in favor of vertical processes. As with vertical mixing, horizontal mixing is caused by localized velocity variations and internal friction, or viscosity. The velocity variations are usually produced by the interactions between the shape of the system and friction, resulting in eddies of varying sizes. Thus, horizontal constituent distributions tend to be broken down by differential advection, which when viewed as an average advection (laterally, or cross-sectionally) is called dispersion.

II.3 ESTUARINE CLASSIFICATION

II.3.1 INTRODUCTION

It is often useful to consider some broad classifications of estuaries, particularly in terms of features and processes which enable us to analyze them in terms of simplified approaches. The most commonly used groupings are based on geomorphology, stratification, circulation patterns, and time scales.

II.3.2 GEOMORPHOLOGICAL CLASSIFICATION

Over the years, a systematic structure of geomorphological classification has evolved. Dyer (1973) and Fischer, et al. (1979) identify four groups:

- Drowned river valleys (coastal plain estuaries),
- Fjords
- Bar-built estuaries, and
- Other estuaries that do not fit the first three classifications.

Typical examples of North American estuaries are presented in Table II-1.

TABLE II-1. TOPOGRAPHIC ESTUARINE CLASSIFICATION

Type	Dominant Long-Term Process	Degree of Stratification	Examples
Coastal Plain	River Flow	Moderate	Chesapeake Bay, MD/VA James River, VA Potomac River, MD/VA Delaware Estuary, DE/NJ New York Bight, NY
Bar Built	Wind	Vertical	Little Sarasota Bay, FL Apalachicola Bay, FL Galveston Bay, TX Roanoke River, VA Albemarle Sound, NC Pamlico Sound, NC
Fjords	Tide	High	Alberni Inlet, B.C. Silver Bay, AL Puget Sound, WA
Other Estuaries	Various	Various	San Francisco Bay, CA Columbia River, WA/OR

Coastal plain estuaries are generally shallow with gently sloping bottoms, and depths increasing uniformly towards the mouth. Such estuaries have usually been cut by erosion and are drowned river valleys, often displaying a dendritic pattern fed by several streams. A well-known example is Chesapeake Bay. Coastal plain estuaries are usually moderately stratified (particularly in the old river valley section) and can be highly influenced by wind.

Bar built estuaries are bodies of water enclosed by the deposition of a sand bar off the coast through which a channel provides exchange with the open sea, usually servicing rivers with relatively small discharges. These are usually unstable estuaries, subject to gradual seasonal and catastrophic variations in configuration. Many estuaries in the Gulf Coast and Lower Atlantic Regions fall into this category. They are generally a few meters deep, vertically well mixed and highly influenced by wind.

Fjords are characterized by relatively deep water and steep sides, and are generally long and narrow. They are usually formed by glaciation, and are more typical in Scandinavia and Alaska than the contiguous United States. There are examples along the Northwest Pacific Coast such as Alberni Inlet in British Columbia and Puget Sound. The freshwater streams that feed a fjord generally pass through rocky terrain. Little sediment is carried to the estuary by the streams, and thus the bottom is likely to be a clean rocky surface. The deep water of a fjord is distinctly cooler and more saline than the surface layer, and the fjord tends to be highly stratified.

The remaining estuaries not covered by the above classification are usually produced by tectonic activity, faulting, landslides, or volcanic eruptions. An example is San Francisco Bay which was formed by movement of the San Andreas Fault System (Dyer, 1973).

II.3.3 STRATIFICATION

A second method of classifying estuaries is by the degree of observed stratification, and was developed originally by Pritchard (1955) and Cameron and Pritchard (1963). They considered three groupings (Figure II-6):

- The highly stratified (salt wedge) type
- Partially mixed estuary
- Vertically homogeneous estuary

Such a classification is intended for the general case of the estuary influenced by tides and freshwater inflows. Shorter term events, such as strong winds, tend to break down highly stratified systems by inducing greater vertical mixing. Examples of different types of stratification are presented in Table II-2.

In the stratified estuary (Figure II-6a), large freshwater inflows ride over saltier ocean waters, with little mixing between layers. Averaged over a tidal cycle, the system usually exhibits net seaward movement in the freshwater layer, and net landward movement in the salt layer, as salt water is entrained into the upper layer. The Mississippi River Delta is an example of this type of estuary.

As the interfacial forces between the saltwater and overlying freshwater become great enough to partially break down the density differences, the system becomes partially stratified, or partially well-mixed (Figure II-6b). Tidal flows are now usually much greater than river flows, and flow reversals in the lower layer may still be observed, although they are generally not as large as for the highly stratified system. Chesapeake Bay and the James River estuary are examples of this type.

In a well mixed system (Figure II-6c), the river inflow is usually very small, and the tidal flow is sufficient to completely break down the stratification and thoroughly mix the system vertically. Such systems are

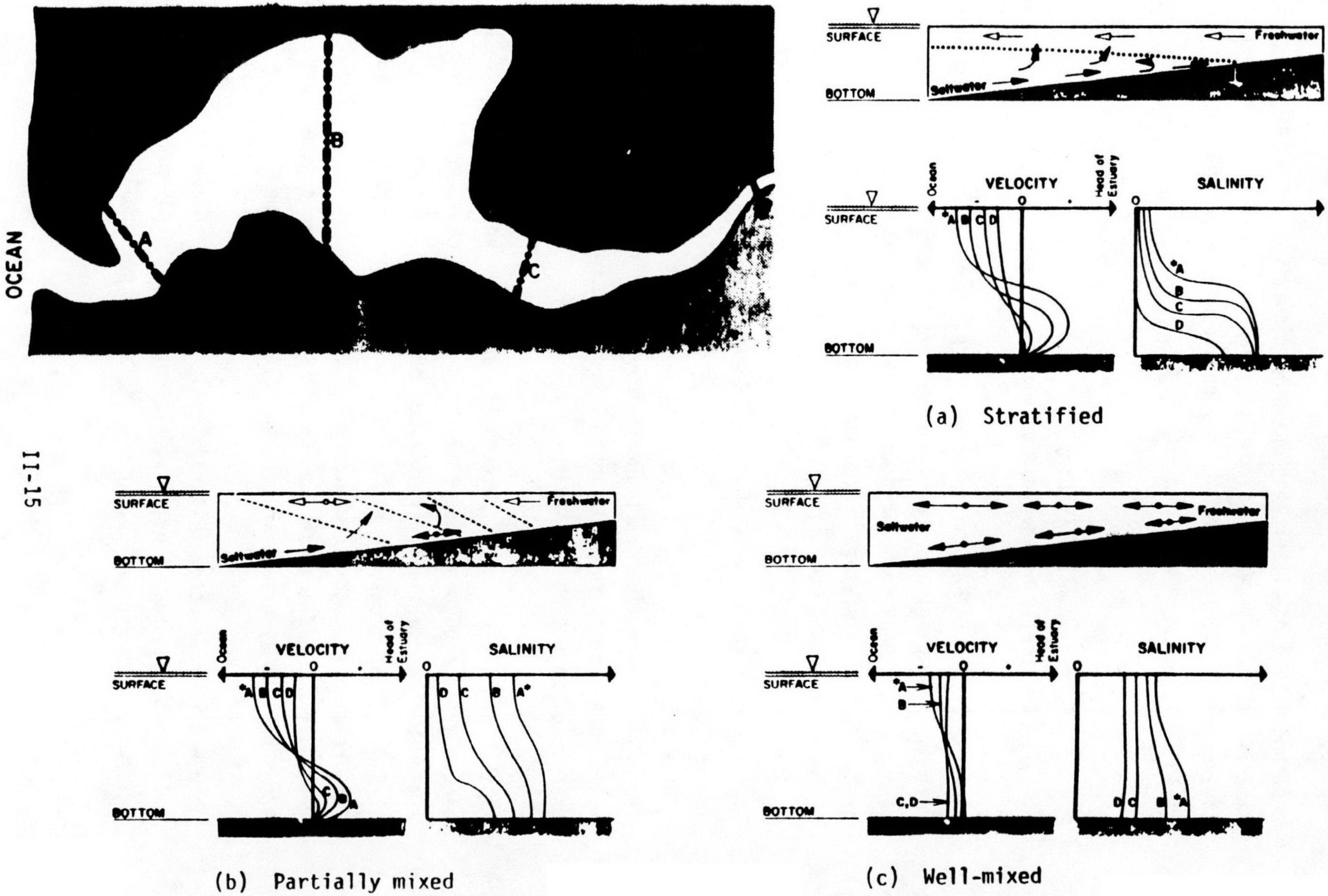


Figure II-6. Classification of Estuarine Stratification.

TABLE II-2. STRATIFICATION CLASSIFICATION

Type	River Discharge	Examples
Highly Stratified	Large	Mississippi River, LA Mobile River, AL Puget Sound, WA
Partially Mixed	Medium	Chesapeake Bay, MD/VA James Estuary, VA Potomac River, MD/VA
Vertically Homogeneous	Small	Delaware Bay, DE/NJ Raritan River, NJ Biscayne Bay, FL Tampa Bay, FL San Francisco Bay, CA San Diego Bay, CA

generally shallow, so that the tidal amplitude to depth ratio is large and mixing can easily penetrate throughout the water column. The Delaware and Raritan River estuaries are examples of well-mixed systems.

II.3.4 CIRCULATION PATTERNS

Circulation in an estuary (i.e., the velocity patterns as they change over time) is primarily affected by the freshwater outflow, the tidal inflow, and the effect of wind. In turn, the difference in density between outflow and inflow sets up secondary currents that ultimately affect the salinity distribution across the estuary. The salinity distribution is important in that it affects the distribution of fauna and flora within the estuary. It is also important because it indicates the mixing properties of the estuary as they may affect the dispersion of pollutants and flushing properties. Additional factors such as friction forces and the size and geometry of the estuary contribute to the circulation patterns.

The complex geometry of estuaries, in combination with the presence of, wind, the effect of the earth's rotation (Coriolis effect), and other effects, often results in residual currents (i.e., of longer period than the tidal cycle) that strongly influence the mixing processes in estuaries. For example, a uniform wind over the surface of an estuary produces a net wind drag which may cause the center of mass of the water in the estuary to be displaced toward the deeper side. Hence a torque is induced causing the water mass to rotate.

In the absence of wind, the pure interaction of tides and estuary geometry may also cause residual currents. For example, flood flows through narrow inlets set up so-called tidal jets, which are long and narrow as compared to the ebb flows which draw from a larger area of the estuary, thus forcing a residual circulation from the central part of the estuary to the sides (Stommel and Farmer, 1952). The energy available in the tide is in part extracted to drive regular circulation patterns whose net result is similar to what would happen if pumps and pipes were installed to move water about in circuits. This is why this type of circulation is referred to as "tidal pumping" to differentiate from wind and other circulation (Fisher, et al., 1979).

Tidal "trapping" is a mechanism -- present in long estuaries with side embayments and small branching channels -- that strongly enhances longitudinal dispersion. It is explained as follows. The propagation of the tide in an estuary -- which represents a balance between the water mass inertia, the hydraulic pressure force due to the slope of the water surface, and the retarding bottom friction force -- results in main channel tidal elevations and velocities that are not in phase. For example, high water occurs before high slack tide and low water before low slack tide because the momentum of flow in the main channel causes the current to continue to flow against an opposing pressure gradient. In contrast, side channels which have less momentum can reverse the current direction faster, thus "trapping" portions of the main channel water which are then available for further longitudinal dispersion during the next flood tide.

II.4 TIME SCALES

A time scale is defined as the period of time over which physical/chemical/biological processes act to produce a condition. The consideration of the time scales of the physical processes being evaluated is very important for any water quality study. Short-term conditions are much more influenced by a variety of short-term events which perhaps have to be analyzed to evaluate a "worst case" scenario. Longer term (seasonal) conditions are influenced predominantly by events which are averaged over the duration of that time scale.

The key to any study is to identify the time scale of the impact being evaluated and then analyze the forcing functions over the same time scale. As an example, circulation and mass transport in the upper part of Chesapeake Bay can be wind driven over a period of days, but is river driven over a period of one month or more. Table II-3 lists the major types of forcing functions on most estuarine systems and gives some idea of their time scales.

TABLE II-3. TIME SCALES OF MAJOR PROCESSES

Forcing Function	Time Scale
TIDE	
One cycle	0.5-1 day
Neap/Spring	14 days
WIND	
Thunderstorm	1-4 hours
Frontal Passage	1-3 days
RIVER FLOW	
Thunderstorm	0.5-1 day
Frontal Passage	3-7 days
Wet/Dry Seasons	4-6 months

II.5 GOVERNING EQUATIONS

The equations that describe the dynamics of water circulation and mass transport in an embayment, estuary, bay or coastal sea are the momentum equation, the continuity equation, the mass transport equations for salinity and temperature, and an equation-of-state relating the density of seawater to the local salinity concentration and/or temperature. The fate of water quality constituents is also governed by the mass transport equation, with the addition of terms to handle chemical kinetics.

Two basic assumptions usually govern the form of these equations: (1) the fluid may be assumed to be incompressible; and (2) flows are nearly horizontal. These assumptions imply that the modeler may neglect compressible effects and vertical accelerations, and may specify the vertical momentum balance by the hydrostatic pressure equation. With these assumptions, and using the Boussinesq approximation applied to the pressure term, the equations may be formed as follows (Leendertse, et al., 1973):

the momentum equations:

$$\frac{\partial u}{\partial t} + \frac{\partial(u^2)}{\partial x} + \frac{\partial(uv)}{\partial y} + \frac{\partial(uw)}{\partial z} - fv + \frac{1}{\rho}\frac{\partial p}{\partial x} = \frac{1}{\rho}\left(\frac{\partial\tau_{xx}}{\partial x} + \frac{\partial\tau_{xy}}{\partial y} + \frac{\partial\tau_{xz}}{\partial z}\right) \quad \text{(II-1)}$$

$$\frac{\partial v}{\partial t} + \frac{\partial(uv)}{\partial x} + \frac{\partial(v^2)}{\partial y} + \frac{\partial(vw)}{\partial z} + fu + \frac{1}{\rho}\frac{\partial p}{\partial y} = \frac{1}{\rho}\left(\frac{\partial\tau_{yx}}{\partial x} + \frac{\partial\tau_{yy}}{\partial y} + \frac{\partial\tau_{yz}}{\partial z}\right) \quad \text{(II-2)}$$

$$\frac{\partial p}{\partial z} + \rho g = 0 \quad \text{(II-3)}$$

the continuity equation:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad \text{(II-4)}$$

the mass transport equation:

$$\frac{\partial c}{\partial t} + \frac{\partial(uc)}{\partial x} + \frac{\partial(vc)}{\partial y} + \frac{\partial(wc)}{\partial z} = \frac{\partial(D_x \frac{\partial c}{\partial x})}{\partial x} + \frac{\partial(D_y \frac{\partial c}{\partial y})}{\partial y} + \frac{\partial(D_z \frac{\partial c}{\partial z})}{\partial z} + r_p \quad \text{(II-5)}$$

and an equation of state in the general form:

$$\rho = \text{function } (s, T) \tag{II-6}$$

where x,y,z = right-hand Cartesian coordinates, with z directed upward (i.e., "x" indicates longitudinal direction, "y" indicates lateral direction, and "z" indicates vertical direction),

t = time, (T),

u, v, w = x, y, z components of the instantaneous velocity, (L/T),

f = Coriolis parameter, (1/T),

ρ = density, (M/L^3),

τ_{ij} = ij component of stress tensor where i, j = x, y, z, (M/LT^2),

p = pressure, (M/LT^2),

g = acceleration due to gravity, (L/t^2),

c = constituent concentration, (M/L^3),

D_x, D_y, D_z = components of diffusion coefficient, (L^2/T),

r_p = source/sink term, (M/TL^3),

s = salinity, ($^\circ$/$\circ\circ$), and

T = temperature, (degrees).

II.6 REDUCING DIMENSIONS

Solutions of the full three-dimensional governing equations of motion and mass transport are always expensive in terms of computer time and other resources, and frequently are more elegant than is necessary to simulate the system being analyzed. Most numerical models simplify these equations either by eliminating spatial dimensions considered not to be important, by time averaging (usually over a tidal cycle), or else by neglecting some of the terms, such as the non-linear convective acceleration terms. The most frequent simplification is a reduction in the number of spatial dimensions modelled. One of three simplifications are used:

- vertical averaging,
- lateral averaging, or
- cross-sectional averaging.

In addition, there are variations to these, such as layer averaging in which the vertical (or lateral) direction is divided into a series of layers over which solution variables are assumed to be constant.

As an example, the most common form of estuarine model simplification is vertical averaging. Equations (II-1)-(II-5) become
momentum equations:

$$\frac{\partial q_x}{\partial t} + \frac{\partial(q_x u)}{\partial x} + \frac{\partial(q_y u)}{\partial y} - f q_y + \frac{h}{\rho}\frac{\partial p}{\partial x} + \frac{1}{\rho}(\tau_{xs} - \tau_{xb}) \tag{II-7}$$

$$= \frac{\partial(N_H h \frac{\partial u}{\partial x})}{\partial x}$$

$$\frac{\partial q_y}{\partial t} + \frac{\partial(q_x v)}{\partial x} + \frac{\partial(q_y v)}{\partial y} + f q_x + \frac{h}{\rho}\frac{\partial p}{\partial y} + \frac{1}{\rho}(\tau_{ys} - \tau_{yb}) \tag{II-8}$$

$$= \frac{\partial(N_H h \frac{\partial v}{\partial y})}{\partial y}$$

continuity equation:

$$\frac{\partial \eta}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0 \tag{II-9}$$

and mass transport equation:

$$\frac{\partial(hc)}{\partial t} + \frac{\partial(q_x c)}{\partial x} + \frac{\partial(q_y c)}{\partial y} \tag{II-10}$$

$$= \frac{\partial(E_H h \frac{\partial c}{\partial x})}{\partial x} \quad \frac{\partial(E_H h \frac{\partial c}{\partial y})}{\partial y} - Khc + hr_p$$

where

q_x, q_y = x-, y-components of flow per unit width, (L^2/T),

u, v = x-, y- components of velocity, (L/T),

f = Coriolis parameter, $(1/T)$,

ρ = density, (M/L^3),

p = pressure, (M/LT^2),

τ_{xs}, τ_{ys} = x-, y-components of surface shear, (M/LT^2),

τ_{xb}, τ_{yb} = x-, y-components of bottom shear, (M/LT^2),

N_H = horizontal momentum transfer coefficient, (L^2/T),

η = surface elevation above datum, (L),

c = constituent concentration,

E_H = horizontal dispersion coefficient, (L^2/T),

K = decay coefficient, $(1/T)$,

x, y = horizontal directions, (L), and

t = time, (T).

In Equation (II-10), the variable, c, can represent salinity, temperature, non-conservative constituents, or water quality variables.

In reducing dimensions, it is important to remember what the solution variables represent. Any form of numerical integration, or averaging, produces variables which are averaged over the dimension of integration. In the above example, Equations (II-7)-(II-10), the resulting velocities are depth-averaged, and as such exhibit no variation with depth. If the system being modelled exhibits vertical variability that is considered to be significant, then it is inappropriate to use this type of model.

More often than not, field data can guide the modeler as to the appropriateness of the simplification used. As an example, many river estuaries are simulated using one-dimensional (cross-sectional average) models. These types of models assume that velocities are cross-sectionally uniform. However, comparisons with field data may show observed velocities which are 2 or 3 times greater than those simulated (e.g., Aldrich, et al., 1983). This is because current meters are usually placed in the deeper, swifter parts of the river and may measure maximum flow, rather than average flows as predicted by the models.

II.7 TIDAL AVERAGING

A different reduction in numerical model complexity is found by performing time averages over the tidal cycle period, T. This eliminates the unsteady, non-uniform flows in the estuary, and replaces them with non-tidal or residual flows. This process is summarized in Harleman (1971).

Consider, for example, the unsteady, non-uniform, one-dimensional, mass transport equation:

$$A \frac{\partial c}{\partial t} + Q \frac{\partial c}{\partial x} = \frac{\partial}{\partial x} (AE_L \frac{\partial c}{\partial x}) + Ar_p - KAc \qquad \text{(II-11)}$$

where

A = cross sectional area, (L^2),
Q = flow, (L^3/T),
E_L = longitudinal dispersion coefficient, (L^2/T), and
K = decay coefficient.

This equation can be time averaged to give (Harleman, 1971):

$$\overline{A} \frac{\partial \overline{c}}{\partial t} + Q_R \frac{\partial \overline{c}}{\partial x} = \frac{\partial}{\partial x}(\overline{AE}_L \frac{\partial \overline{c}}{\partial x}) + \overline{Ar}_p \qquad \text{(II-12)}$$

where

Q_R = river flow, (L^3/T), and
overbar = time average over a tidal cycle.

For a steady-state river flow (Q_f = constant) and a conservative substance ($\bar{r}_p = 0$), the steady-state flow of Equation (II-12) is (Stommel, 1953):

$$Q_R \frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial x} (\overline{AE}_L \frac{\partial \bar{c}}{\partial x}) \tag{II-13}$$

Another way to consider Equation (II-12) is as a slack water approximation (O'Connor and Di Toro, 1964; O'Connor, 1965) in which the concentration, is calculated at successive high or low water slack tides:

$$A_s \frac{\partial c_s}{\partial t} + Q_R \frac{\partial c_s}{\partial x} = \frac{\partial}{\partial x} (A_s \bar{E}_s \frac{\partial c_s}{\partial x}) + A_s r_p - K_s A_s c \tag{II-14}$$

where the subscript, denotes values at slack water.

In each of these approaches, it is important to understand what is, and what is not represented by the equations. Both approaches are essentially the same, with the exception of the time varying term in Equation (II-14), and represent time averages over the tidal cycle, T. This means that fluctuations of transport phenomena within the tidal cycle cannot be resolved, and as such are treated using the dispersion term, E_L or E_s, both of which must be larger than the unsteady coefficient, E_L, in Equation (II-11).

This can be a very useful approach, and not just in terms of computational savings, provided that the system responds in an appropriate manner and important information is not lost. At one extreme, consider the case of a tidal regime with no river flow, $Q_R = 0$. Then all advective processes are lost and replaced with a tidally-averaged dispersion coefficient.

II.8 DISPERSION COEFFICIENTS

The mass transport equation, Equation (II-5) contains dispersion coefficients, D_x, D_y, D_z, which represent a combination of sub-grid processes within the numerical discretization in the three principle directions. The common forms of these coefficients and their representations after spatial and temporal averaging is worth some discussion. We will also discuss briefly their relative impacts within more common numerical model schemes. An excellent background discussion of mixing processes can be found in Fischer et al. (1979).

In three-dimensional models, one of two approaches is often used. For near-field models, such as close to ocean outfalls, it is common to assign constant values to the coefficients:

$$D_x = C_1, \; D_y = C_2, \; D_z = C_3 \qquad \text{(II-15)}$$

Further, at least horizontal isotropy is often assumed, $C_1 = C_2$. In far field models, where the entire depth of flow and perhaps stratification become important, the vertical coefficient may be made a function of internal flow parameters, usually characterized by the local or bulk Richardson numbers:

e.g., (Leendertse et al., 1975)

$$D_z = D_o \, e^{-3R_i} \qquad \text{(II-16)}$$

where D_o = vertical dispersion coefficient for neutral stability condition, (L^2/T), and

R_i = local Richardson number

$$= \frac{g(\partial\rho/\partial z)}{\rho(\partial u/\partial z)^2}$$

For two-dimensional, laterally-averaged models, the approach is usually to use a three dimensional formulation, and simply drop the lateral coefficient. Model calibration provides any further adjustment to coefficient values that reflect lateral averages.

In most two-dimensional, vertically-averaged models, the horizontal coefficients are usually specified as constants, and in many cases, isotropy is assumed.

Perhaps the most critical selection for model dispersion coefficients is the category of one-dimensional models--both dynamic and steady-state. For models that include a dynamic description of one-dimensional hydrodynamic processes, most coefficients are based on a formulation of the form:

$$E_L = KR|u| \qquad \text{(II-17)}$$

where E_L = longitudinal dispersion coefficient, (L^2/T),
K = dimensionless dispersion coefficient,
R = hydraulic radius, (L), and
u = velocity, (L/T)

that follows from the work of Taylor (1954) and Elder (1959). Similar forms have been derived by Harleman (1964 and 1971, respectively):

$$E_L = 77\ n|u|R^{5/6} \qquad \text{(II-18)}$$
$$E_L = 100\ n|u_{max}|R^{5/6}$$

where n = Manning's roughness coefficient (0.02-0.035, typically), and
u_{max} = maximum tidal velocity, (L/T).

When the modeler applies time-averaging in the governing equations, however, the choice of dispersion coefficients becomes much more difficult. This is because the dispersive terms in the resulting time-average mass-transport equation now contain representations of processes whose time scales are less than the time over which averaging is performed. The most common form of time averaging is over the tidal period, T. In this case, the dispersive terms contain tidal fluctuations of velocity and constituent mass.

Selection of dispersion coefficients, E_L^T, in one-dimensional, tidally-averaged models is usually performed in one of three ways:

1. E_L^T = constant (space, time) (II-19)

2. E_L^T = constant (time) (II-20)

3. $E_L^T = KRQ_R/A$ (II-21)

In the first method, a uniform coefficient is selected over time and space, and calibrated to best fit observations. This is usually done when there is little data for calibration, and often leads to poor results when adequate data become available for comparison.

In the second method, the coefficient is allowed to vary in space only, and is held constant through time. Using this approach increases the number of unknown coefficients to the number of boxes or nodes in the system, resulting in increased difficulty in calibration, though generally more accurate calibrations.

The third approach, or variations thereof, attempts to reduce the number of unknowns again to one--that is, the dimensionless coefficient, K. In doing this, the approach is to relate the coefficient, E_L^T, to some property (e.g., RQ_R/A in Equation (II-21)) that describes the variability found in the system in trying to match the form of Equation (II-20). The objective is to reduce the number of unknowns and yet achieve accurate calibrations as is theoretically possible with Equation (II-20). In fact, even more accurate calibrations may result if multiple data sets are available, because the form of Equation (II-21) is also variable through time as Q_R varies.

Unfortunately, in many systems, coefficients based on the form of Equation (II-12) fail to achieve satisfactory results because the form of explicit dependence (river flow, Q_R, in this case) is the wrong measure of system variability. Such an approach works well for rivers where it was originally conceived and tested, and probably works well for river dominated tidal estuaries. However, let us explore the case in which the tidal estuary is dominated by the tide. To simplify the analysis, we will make the following assumptions:

- o the estuary is short enough that the water surface is almost horizontal,
- o the form of E_L^T by Equation (II-17) is adequate to describe tidally-varying coefficients, and
- o tidal forcing given by:

$$\eta = a \cos(wt) \tag{II-22}$$

where η = tidal elevation above MSL, (L),
a = tidal amplitude, (L)
w = tidal frequency = $2\pi/T$, (1/T),
T = tidal period, (T), and
t = time, (T).

These assumptions are generally reasonable for an estuary in which a one-dimensional, mass transport model can be applied. From these assumptions, the cross-sectional averaged velocity (u, positive downstream) can be found from the continuity equation alone (Walton, 1978):

$$u = (Q_R + A_{ws} \frac{\partial \eta}{\partial t})/A = (Q_R - A_{ws}\, aw \sin(wt))/A \tag{II-23}$$

where A_{ws} = upstream area of water surface, (L^2), and
A = cross-sectional area, (L^2).

The time-varying dispersion coefficient, E_L, from Equation (II-17) is then:

$$E_L = KR|Q_R - A_{ws}\, aw \sin(wt)|/A \tag{II-24}$$

This distribution is shown schematically in Figure II-7, along with the resulting velocity distribution.

The further assumption is now made that the tidal-time average of the unsteady mass transport equation leads to a dispersion coefficient, E_L^T, that is proportional to the time average of E_L from Equation (II-24) (the coefficient of proportionality reflects the effects of the constituent gradient, $\partial c/\partial x$ over the tidal cycle). This is reasonable when one considers the form of the coefficients chosen for many one-dimensional, steady-state models. From Figure II-7, the velocity goes to zero at

$$t_1 \text{ and } t_2 = \frac{1}{w} \sin^{-1}\left[\frac{Q_R}{awA_{ws}}\right] \text{ for } 0 \leq t < T \tag{II-25}$$

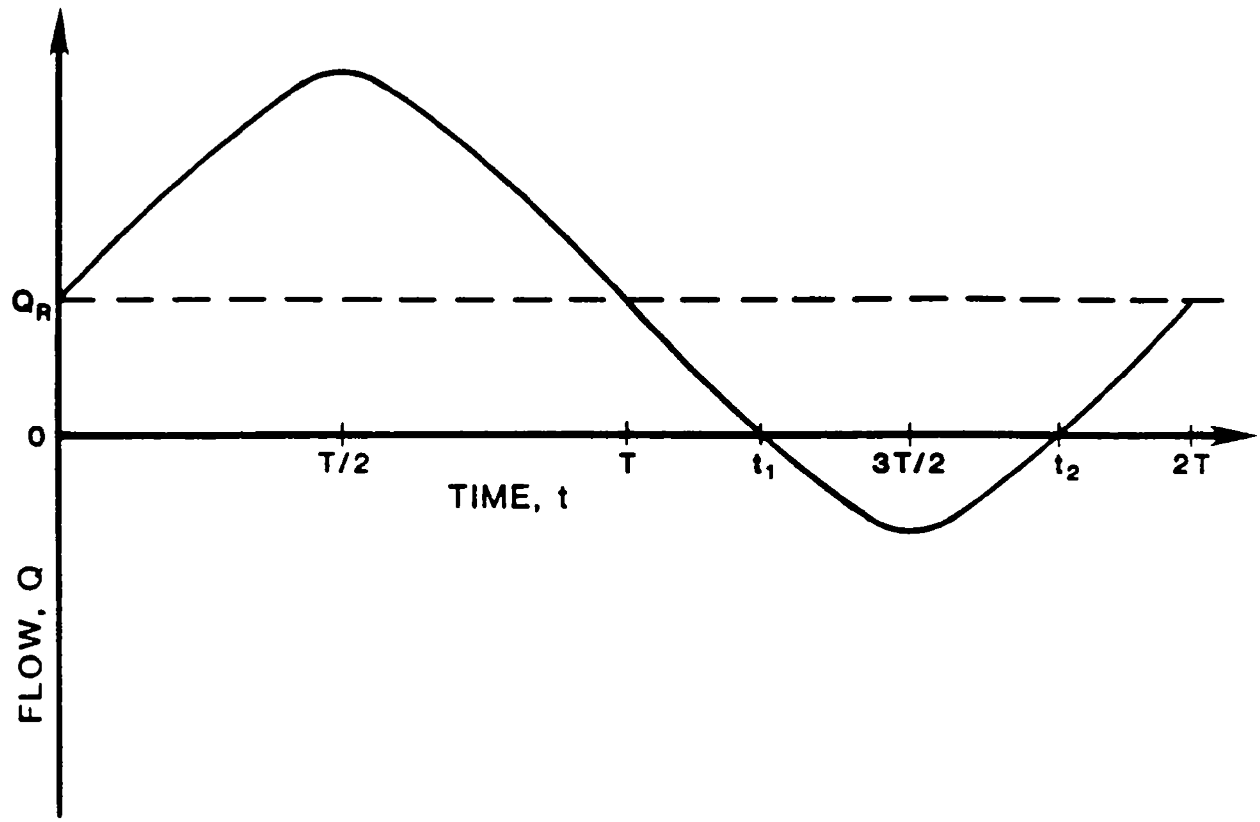


Figure II-7 TIME VARYING AND RESIDUAL TIDAL FLOWS and thus:

$$E_L^T = \frac{1}{T}\left[\int_0^{t_1} E_L dt - \int_{t_1}^{t_2} E_L dt + \int_{t_2}^{T} E_L dt\right] \tag{II-26}$$

$$= \frac{KR}{TA}\left[Q_R(T+2t_1 - 2t_2) + 2aA_{ws}(1+\cos(wt_1) - \cos(wt_2))\right]$$

If Q_R is sufficiently large that the velocity is always positive (downstream), then t_1 and t_2 do not exist, and the steady-state dispersion coefficient is given by:

$$E_L^T = KRQ_R/A \tag{II-27}$$

At the other extreme, if Q_R is small, then $t_1 = 0$, $t_2 = T/2$ and Equation (II-26) reduces to:

$$E_L^T = \frac{4aA_{ws}\ KR}{TA} \tag{II-28}$$

Examining the results of Equations (II-26)-(II-28), one can see the difficulty in obtaining dispersion coefficients for a steady-state model (even assuming that such a model is a true representation of natural processes). If the river flow dominates the system everywhere, then the use of Equation (II-27) is justified. However, even in cases where there is a strong river inflow, such as in the Potomac River, this formulation may only apply in the upstream portion where Q_R dominates. In the downstream section of the Potomac, tidal flows dominate and one might expect the relationship of Equation (II-28) to hold. Between these two sections, in which Equation (II-25) is satisfied, one might expect a balance between river and tidal influences. In this region, Equation (II-26) could be used as a guide to coefficient selection, or a laborious calibration could be followed with coefficients specified at each node or box of the system.

II.9 DECAY COEFFICIENTS

Non-conservative mass transport and water quality models contain a decay or reaction kinetics term, of the form -Kc, where K is a decay coefficient and c is the constituent concentration. A non-conservative mass transport model takes the form:

$$\frac{\partial c}{\partial t} + R = -Kc \tag{II-29}$$

and a water quality model may have the general form:

$$\frac{\partial c}{\partial t} + R = -Ks \tag{II-30}$$

where c = constituent concentration,
R = other terms of the equation,
K = decay rate, (1/T), and
s = constituent influencing decay.

These forms are termed "first order" reactions and serve to describe such processes in the majority of numerical models. Higher order reaction kinetics are occasionally used in more complex water quality models.

Formulation of decay or reaction kinetics relationships in non-steady models is generally not a problem. Usually, the main concern is over numerical stability, through the selection of a time step, Δt, in an explicit model simulation (most models use explicit schemes allowable time step in which there is a maximum for numerical stability). If we neglect R in Equation (II-29) for the moment, an explicit approximation to the remaining terms is:

$$c^{n+1} = c^{n}(1 - K\Delta t) \tag{II-31}$$

where n denotes time level.

From Equation (II-31) one can see an obvious stability condition, often overlooked, that:

$$t \leq 1/K \tag{II-32}$$

It is also interesting to note that Equation (II-29), with R = 0, can be solved directly:

$$c^{n+1} = c^{n} e^{-K\Delta t} \tag{II-33}$$

which will always be stable. Unfortunately, the stability condition on Equation (II-30) is not as obvious, but the condition of Equation (II-32) should serve as a general guide.

There is a more fundamental problem when one looks at steady-state models, particularly for high decay rates. Consider the problem of fecal coliform fate modeling in which the decay coefficient represented by T_{90} (= 2.3/K) was much less than the tidal period T. Tidally averaged models could not produce the same pattern of maximum coliform values, and certainly not their occurrence through time, as for an unsteady model.

Intuitively, one might expect a criterion, D, to be based on a ratio of the T_{90} value of the non-conservative constituent or critical water quality parameter, to the flushing time, F:

$$D = T_{90}/F \tag{II-34}$$

As $D \rightarrow 0$ for a conservative substance, a steady-state model might be applicable. As $D \geq D_c$, where D_c is a threshold value to be determined, decay becomes important, and an unsteady model should be used. At present, there is no means to determine appropriate values of D_c for given tolerances of solutions.

SECTION III

WATER QUALITY PROCESSES

III.1 GENERAL

There are many chemical and biological actions and interactions that constitute water quality processes. The following section will describe a variety of biochemical processes, however, the most critical water quality parameters to be considered as part of the wasteload allocation process are dissolved oxygen, nutrients, chlorophyll-a, coliforms and toxicants.

Dissolved oxygen (DO) is an important water quality indicator for all fisheries uses. The DO concentration in bottom waters is the most critical indicator of survival and/or density and diversity for most shellfish and an important indicator for finfish. DO concentrations at mid-depth and surface locations are also important indicators for finfish. Assessments of DO impacts should consider the relative contributions of three different sources of oxygen demand: (a) net photosynthesis/respiration demand from phytoplankton, perriphyton and rooted aquatic plants; (b) water column demand due to decay of suspended organic matter and chemical reactions; and (c) benthic oxygen demand. Assessments of the significance of each oxygen sink can be used to evaluate the requirements for achieving the required degree of pollution control.

The nutrients of concern in the estuary are nitrogen and phosphorus. Their sources typically are discharges from sewage treatment plants and industries, and runoff from urban and agricultural areas. Increased nutrient levels lead to phytoplankton blooms and a subsequent reduction in DO levels. In addition, algal blooms decrease the depth to which light is able to penetrate, thereby adversely affecting submerged aquatic vegetation populations in the estuary. Nutrient enriched waters can also produce increased perriphyton growth on submerged aquatic vegetation which blocks the light and kills the vegetation.

Sewage treatment plants are typically the major source of nutrients to estuaries in urbanized areas. Agricultural land uses and urban land uses, however, represent significant nonpoint sources of nutrients. Often wastewater treatment plants are the major source of phosphorus loadings while nonpoint sources tend to be major contributors of nitrogen. In estuaries located near highly urbanized areas, municipal discharges probably will dominate the point source nutrient contributions. Thus, it is important to base control strategies on an understanding of the sources of each type of nutrient, both in the estuary and in its feeder streams.

The method of choice for controlling primary productivity in the tidal fresh zone of an estuary (upper estuary), which is phosphorus limited, is phosphorus removal from municipal discharges, because point sources of nutrients are typically much more amenable to control than nonpoint sources, and because phosphorus removal from municipal wastewater discharges is less expensive than nitrogen removal. However, the nutrient control programs for the upper estuary can have an adverse effect on control of phytoplankton growth in the lower estuary (i.e., near the mouth) where nitrogen is typically the critical nutrient for eutrophication control. This is because the reduction of phytoplankton concentrations in the upper estuary will reduce the uptake and settling of the non-limiting nutrient which is typically nitrogen, thereby resulting in increased transport of nitrogen through the upper estuary to the lower estuary where it is the limiting nutrient for algal growth. The result is that reductions in algal blooms within the upper estuary due to the control of one nutrient (phosphorus) can result in increased phytoplankton concentrations in the lower estuary due to higher levels of the uncontrolled nutrient (nitrogen). Thus, tradeoffs between nutrient controls for the upper and lower estuary should be considered in performing wasteload allocations.

Chlorophyll-a, because it is easy to measure, is the most popular indicator of algal concentrations and nutrient overenrichment which in turn can be related to diurnal DO depressions due to algal respiration. Typically, the control of phosphorus levels can limit algal growth in the upper end of the estuary, while the control of nitrogen levels can limit algal growth near the mouth of the estuary. However, these relationships are dependent upon factors such as N:P ratios and light penetration potential, which can vary from one estuary to the next due to natural or man-generated turbidity in the water column, thereby producing different limiting conditions within a given estuary. Excessive phytoplankton concentrations, as indicated by chlorophyll-a levels, can cause adverse DO impacts such as: (a) wide diurnal variations in surface DO's due to daytime photosynthetic oxygen production and nighttime oxygen depletion by respiration; and (b) depletion of bottom DO's through the decomposition of dead algae. Thus, excessive chlorophyll-a levels can deplete the oxygen resources required for bottom water fisheries, exert stress on the oxygen resources of surface water fisheries, and upset the balance of the detrital foodweb in the seagrass community through the production of excessive organic matter. Excessive chlorophyll-a levels also result in shading which reduces light penetration for submerged aquatic vegetation.

The transport, fate, and impact on biota of toxicants such as pesticides, herbicides, heavy metals, and chlorinated effluents are also important factors to consider. The presence of certain toxicants in excessive concentrations in the water column or within bottom sediments can impact fisheries propagation/harvesting and seagrass habitat. This can occur in estuary segments which satisfy water quality criteria for DO, chlorophyll-a, nutrient enrichment, and fecal coliforms.

III.2 BIOCHEMICAL PROCESSES

Several biological and chemical parameters or constituents can be investigated separately because their concentrations are independent of other constituent concentrations. Other constituent concentrations, however, are dependent on the concentrations of other constituents. The following discussion begins with those parameters which are independent and proceeds toward those which are most interdependent.

III.2.1 CONSERVATIVE SUBSTANCES

Conservative substances neither react with other constituents nor do they decay. They are only dependent on the loads from the headwater and tidal boundaries, and from the point and nonpoint contributions to the estuary. Such substances include chlorides, alkalinity, total dissolved solids, total nitrogen, total phosphorus, and sometimes heavy metals. The processes surrounding heavy metals can be very complicated. In model applications, however, they are usually considered as conservative substances.

The kinetic representation for a conservative substance is:

$$\frac{ds}{dt} = 0 \qquad \text{(III-1)}$$

where s = conservative substance.

III.2.2 BIOCHEMICAL OXYGEN DEMAND

The ultimate biochemical oxygen demand (BOD) includes carbonaceous and nitrogenous BOD. Most model applications break up this total into its carbonaceous and nitrogenous components. The nitrogenous component is accounted for within the analysis of the nitrogen series. The change in BOD concentration can be represented by a first order decay rate. If the total carbonaceous and nitrogenous BOD is being considered as one constituent, then the decay rate must reflect the carbonaceous and nitrogenous processes. On the other hand, if nitrogenous BOD is considered separately, then the appropriate carbonaceous rate constant must be selected. BOD decreases can also be attributed to the rate of loss due to settling. The BOD reduced as a function of the decay rate exerts an oxygen demand on the dissolved oxygen in the water column while the BOD loss due to settling becomes a benthic oxygen demand.

The rate of change of BOD is formulated as a first order reaction. If carbonaceous BOD and settling are considered the representation of the BOD decay and settling is:

$$\frac{d(BOD)}{dt} = -K_1(BOD) - \frac{K_3}{d}(BOD) \qquad \text{(III-2)}$$

where

BOD = concentration of carbonaceous BOD,
K_1 = rate of decay of carbonaceous BOD,
K_3 = settling rate of BOD,
d = depth.

III.2.3 FECAL COLIFORMS

Fecal coliforms are affected only by waste input strength and a decay rate. The reduction in fecal coliforms is a function of the coliform die-off rate and the concentration of the coliforms in the water column. The equation that describes the die-off of fecal coliforms (first order kinetics) is:

$$\frac{dE}{dt} = - K_4 E \qquad \text{(III-3)}$$

where

E = concentration of coliforms,
K_4 = coliform die-off rate.

III.2.4 PHOSPHORUS

Sources of phosphorus include wasteload, incremental inflows and benthic deposits. The phosphorus cycle is less complicated than the nitrogen cycle because for a simplistic representation, its only interaction is with algae. This representation does not include interactions with fish, zooplankton, benthic animals, organic sediment and detritus. One approach is to consider only the dissolved orthophosphorus and relate its concentration change to algae growth and respiration, and a benthic source rate.

Another approach would be to consider two components of phosphorus: the non-living organic phosphorus and the orthophosphorus. In this scheme, organic phosphorus is decomposed with first order kinetics to orthophosphorus. Organic phosphorus can also be lost due to settling where it becomes a benthic source of phosphorus. The source of organic phosphorus is from algal respiration. For the second component, orthophosphorus, the source is the decomposed organic phosphorus and the uptake is due to algal growth. Another source of orthophosphorus which could be considered is the release from sediment.

A graphic example of the phosphorus cycle is shown in Figure III-1. The figure presents the various actions and interactions of phosphorus, including not only algae or phytoplankton as discussed above, but also the link to zooplankton which is discussed in a subsequent section.

The decomposition of organic phosphorus to orthophosphorus is represented with first order kinetics; additional loss can be attributed to settling. The source of organic phosphorus is algal respiration. The general formulation is thus:

$$\frac{d(ORGP)}{dt} = - K_5(ORGP) - \frac{K_6}{d}(ORGP) + f_{ap}r_aA \qquad \text{(III-4)}$$

where

ORGP = concentration of organic phosphorus,
K_5 = rate of decomposition of organic phosphorus,
K_6 = settling rate of organic phosphorus,
d = depth,
f_{ap} = fraction of algal biomass which is phosphorus,
r_a = respiration rate of algae,
A = algal biomass concentration.

Orthophosphorus does not decay. However, its sources and sink can be represented by the following formula:

$$\frac{dP}{dt} = K_5(ORGP) - f_{ap}g_aA + \frac{K_7}{d} \qquad \text{(III-5)}$$

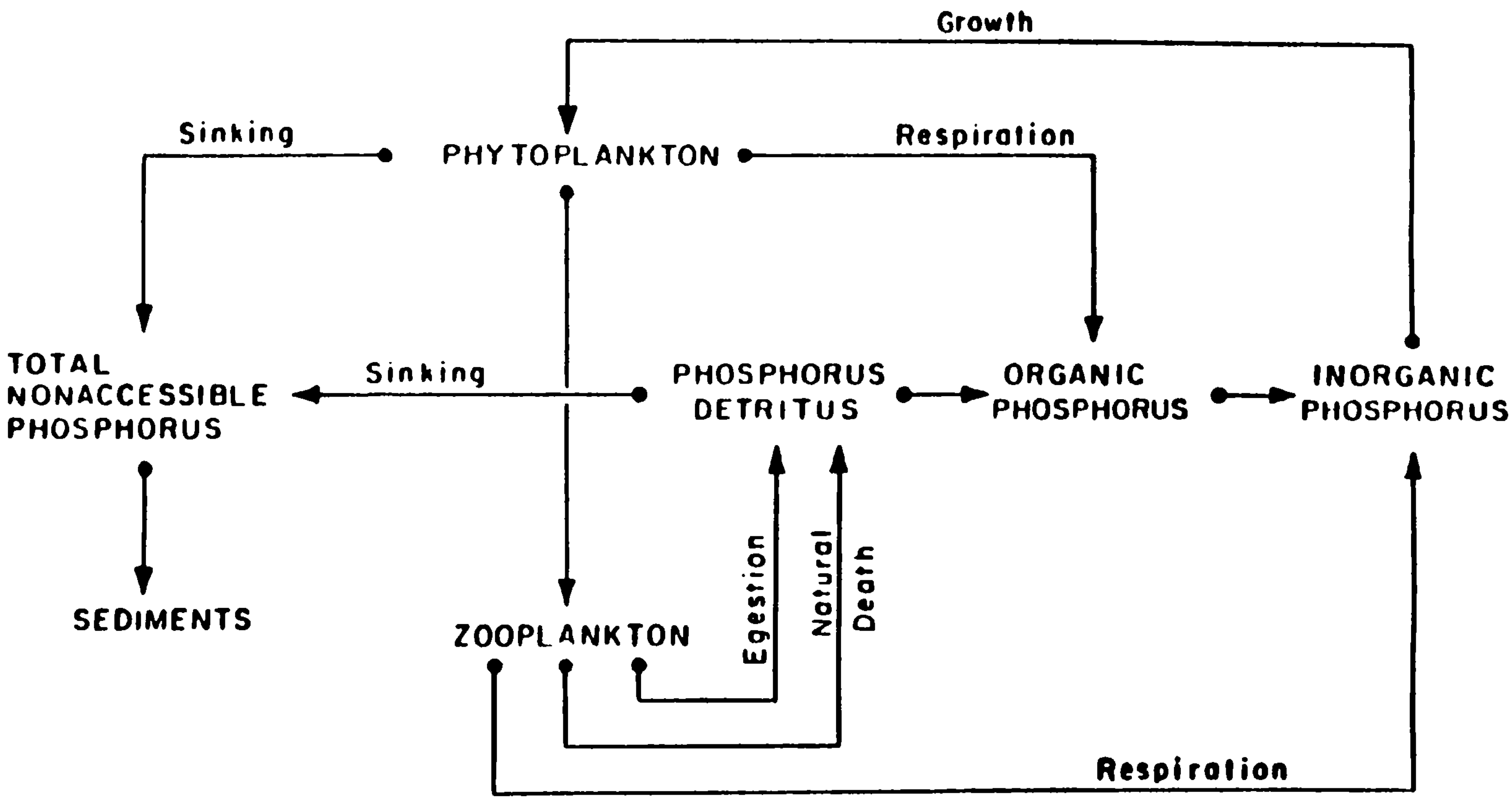


Figure III-1. Phosphorus Cycle (modified after Canale, et al., 1976).

where

P = concentration of orthophosphorus,
K_5 = rate of decomposition of organic phosphorus,
ORGP = concentration of organic phosphorus,
f_{ap} = fraction of algal biomass which is phosphorus,
g_a = specific growth rate of algae,
A = algae concentration,
K_7 = benthic source rate of orthophosphorus,
d = depth.

III.2.5 NITROGEN

The nitrogen cycle can be analyzed simply as its two major components ammonia and nitrate or with more detail considering all four components. For this first case, only ammonia nitrogen and nitrite-nitrate nitrogen are considered. Ammonia nitrogen decays with a first order rate to the sum of nitrite + nitrate and by doing so produces an oxygen demand. This approach is feasible because nitrite serves only as an intermediate product and its oxidation to nitrate is rapid. Under this scheme, a source of ammonia is from respired (dead) algal biomass which is resolubilized as ammonia nitrogen by bacterial action. Another source of ammonia that can be considered is the benthic source. The nitrite-nitrate which is produced from the ammonia decay is reduced as a function of the algal growth.

In a more extensive scheme, organic nitrogen, ammonia nitrogen, nitrite nitrogen, and nitrate nitrogen can be considered separately. Organic nitrogen is decomposed to ammonia using first order kinetics. Settling can also be considered as a loss of organic nitrogen from the water column. The source of ammonia nitrogen is from the decomposed organic nitrogen in the water column and from the benthos. Ammonia is lost through a first order decay rate, settling and uptake during algal growth. (Note that in this scheme, algal growth relies on ammonia as well as nitrate.) Nitrite's source is the decayed ammonia and the nitrite is decayed to nitrate by first order kinetics. The source of nitrate is then a function of the amount of nitrite decayed, and the benthic source rate for nitrate. A sink or reduction of nitrate is the nitrate uptake during algal growth.

An example of the nitrogen cycle is presented in Figure III-2. The figure shows the relationships of the various forms of nitrogen and their link to phytoplankton (algae) as discussed above. Figure III-2 also shows the links to nitrogen detritus and zooplankton which are discussed in a subsequent section.

For the scheme where all four forms of nitrogen are to be considered, the governing transformations are given below.

For Organic Nitrogen:

$$\frac{dORGN}{dt} = - K_8 ORGN - \frac{K_9 ORGN}{d} + f_{an} r_a A \qquad \text{(III-6)}$$

where

ORGN = organic nitrogen,
K_8 = rate of decomposition of organic nitrogen,
K_9 = settling rate of organic nitrogen,
d = depth,
f_{an} = fraction of algal biomass which is nitrogen,
r_a = respiration rate of algae,
A = concentration of algae.

For Ammonia:

$$\frac{dNH3}{dt} = K_8 ORGN + \frac{K_{10}}{d} - K_{11} NH3 - \frac{K_{12}}{d} NH3 - P_a f_{an} g_a A \qquad \text{(III-7)}$$

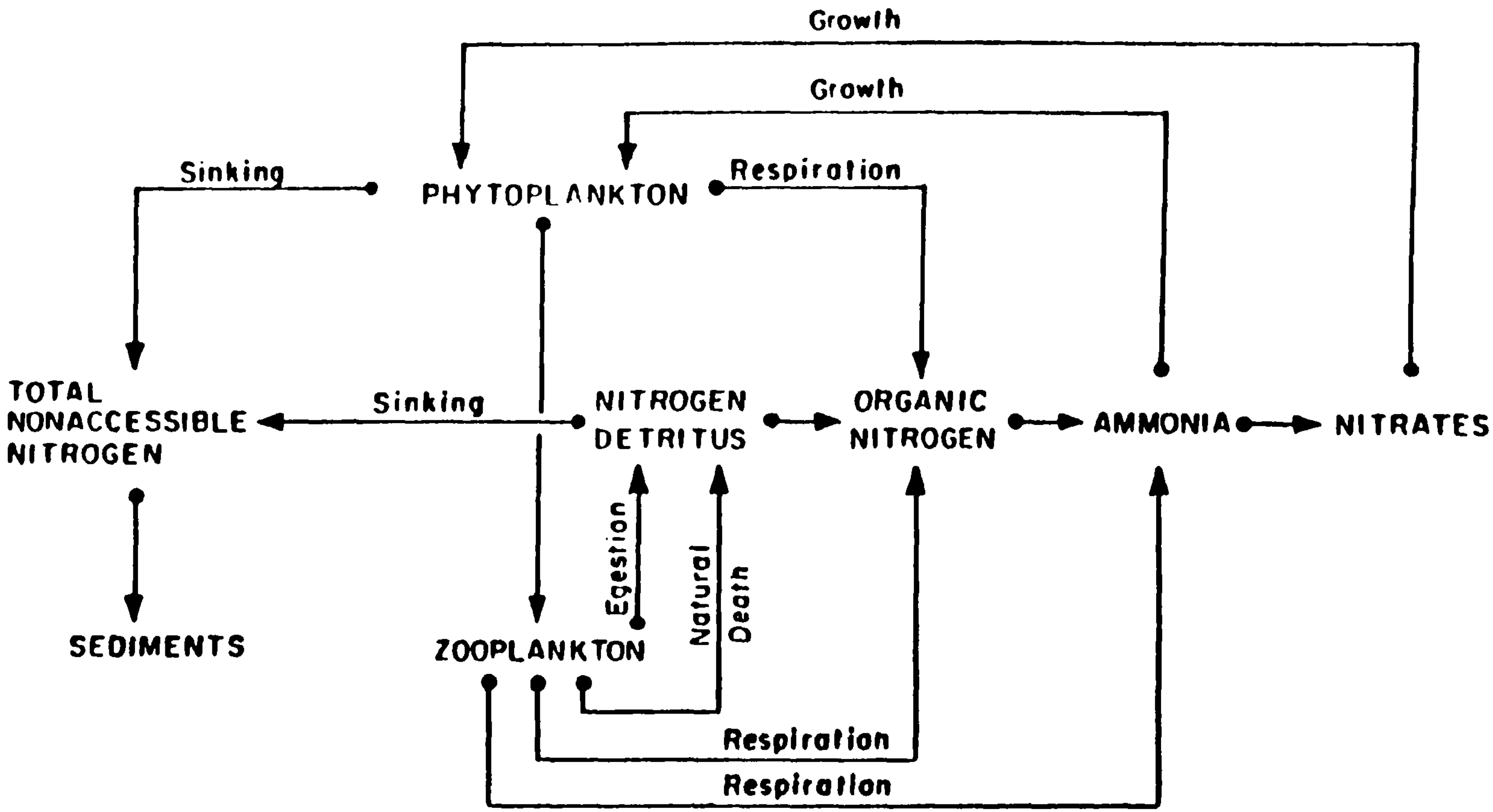


Figure III-2. Nitrogen Cycle (modified after Canale, et al., 1976).

where

$NH3$ = ammonia,
K_8 = rate of decomposition of organic nitrogen,
$ORGN$ = organic nitrogen,
K_{10} = benthic source rate of ammonia,
d = depth,
K_{11} = rate of biological oxidation of ammonia,
K_{12} = settling rate of ammonia,
p_a = fraction of algae biomass that prefers NH3 for growth,
f_{an} = fraction of algal biomass which is nitrogen,
g_a = specific growth rate of algae,
A = concentration of algae.

For Nitrite:

$$\frac{d(NO2)}{dt} = K_{11}(NH3) - K_{13}(NO2) \qquad \text{(III-8)}$$

where

$NO2$ = nitrite concentration,
K_{11} = rate of biological oxidation of ammonia,
$NH3$ = ammonia concentration,
K_{13} = rate of oxidation of nitrite.

For Nitrate:

$$\frac{d(NO3)}{dt} = K_{13}(NO2) - (1-p_a)\ f_{an}g_aA + \frac{K_{14}}{d} \qquad \text{(III-9)}$$

where

$NO3$ = nitrate concentration,
K_{13} = rate of oxidation of nitrite,
$NO2$ = nitrite concentration,
$(1-p_a)$ = fraction of algae that prefers nitrate,

f_{an} = fraction of algae biomass which is nitrogen,

g_a = specific growth rate of algae,

A = algae,

K_{14} = benthic source rate of nitrate.

III.2.6 NITROGEN AND PHOSPHORUS WITHOUT ALGAE, SETTLING OR BENTHIC SOURCES

If algal growth and respiration are not a major concern, then the factors which act as sources or sinks within the nitrogen cycles can be deleted. As for phosphorus, if algal biomass, settling, or benthic release are not considered, then for studying only orthophosphorus it would be considered a conservative substance. If organic phosphorus and orthophosphorus are considered, then the only action would be the loss of organic phosphorus due to its decay rate and the increase of orthophosphorus from the decayed organic phosphorus.

Likewise, if algae, settling or sediment release, which govern the various species of nitrogen are not included, then only the ammonia and nitrite decay rates will produce the different components of the nitrogen cycle.

III.2.7 ALGAE

In many studies, chlorophyll-a is used as an indicator of algal biomass. In modeling, the chlorophyll-a concentration is converted by a factor to the algal biomass concentration. The change in algal biomass concentration can be represented simply by the algal growth as a source, which adds oxygen to the system, and by algal respiration as a loss, which depletes the oxygen in the water column. In addition to these two main processes, algal settling and predation can be considered as sinks for the algal biomass.

Algal production is coupled to the available nutrient supply and the light intensity. In some formulations, to determine the growth rate, a maximum growth rate is multiplied by a light limitation factor, a nitrogen limitation factor, and a phosphorus limitation factor. In others, the maximum growth rate is multiplied by the light limitation factor and the minimum of the nitrogen and phosphorus limitation factors.

The discussion above pertains mainly to green and blue-green algae. In some cases, diatoms may be an important factor in the oxygen balance and the food chain. Diatoms are algae whose cell walls contain silica. They require much more silica than do the other types of algae. The diatoms will uptake dissolved silicon during the growth period and will release silicon during respiration.

A simple equation that governs the growth and production of algae is formulated as follows:

$$\frac{dA}{dt} = g_a A - r_a A \qquad \text{(III-10)}$$

where

A = algae concentration,
g_a = specific growth rate of algae,
r_a = respiration rate of algae.

Two additional processes can be added to account for the loss of algae due to settling and predation. With these two terms, the expanded equation is:

$$\frac{dA}{dt} = g_a A - r_a A - \frac{K_{15}}{d} A - K_{16} A \qquad \text{(III-11)}$$

where (in addition to the terms above)

K_{15} = settling rate for algae
K_{16} = predation rate

As discussed above, the specific growth rate of algae is coupled to the availability of required nutrients and light.

The specific growth rate (g_a) can be determined by the following equation:

$$g_a = g_{amax} L_L \, MIN \, (L_n, L_p) \tag{III-12}$$

where

g_a = specific growth rate of algae,
g_{amax} = maximum specific growth rate of algae,
L_L = light limitation factor,
$MIN \, (L_n, L_p)$ = the minimum value of L_n, the nitrogen limitation factor, and L_p, the phosphorus limitation factor.

The light limitation factor is defined as:

$$L_L = \frac{1}{xd} \; L_n \; \frac{K_L + L}{K_L + Le^{-xd}} \tag{III-13}$$

where

x = light extinction coefficient,
d = depth,
K_L = empirical half saturation constant for light,
L = light intensity.

The nitrogen limitation factor is defined as:

$$L_n = \frac{(NH3 + NO3)}{(NH3 + NO3) + K_n} \tag{III-14}$$

where

NH3 = ammonia concentration,
NO3 = nitrate concentration,
K_n = empirical half saturation constant for nitrogen.

The phosphorus limitation factor is defined as:

$$L_p = \frac{P}{P + K_p} \qquad \text{(III-15)}$$

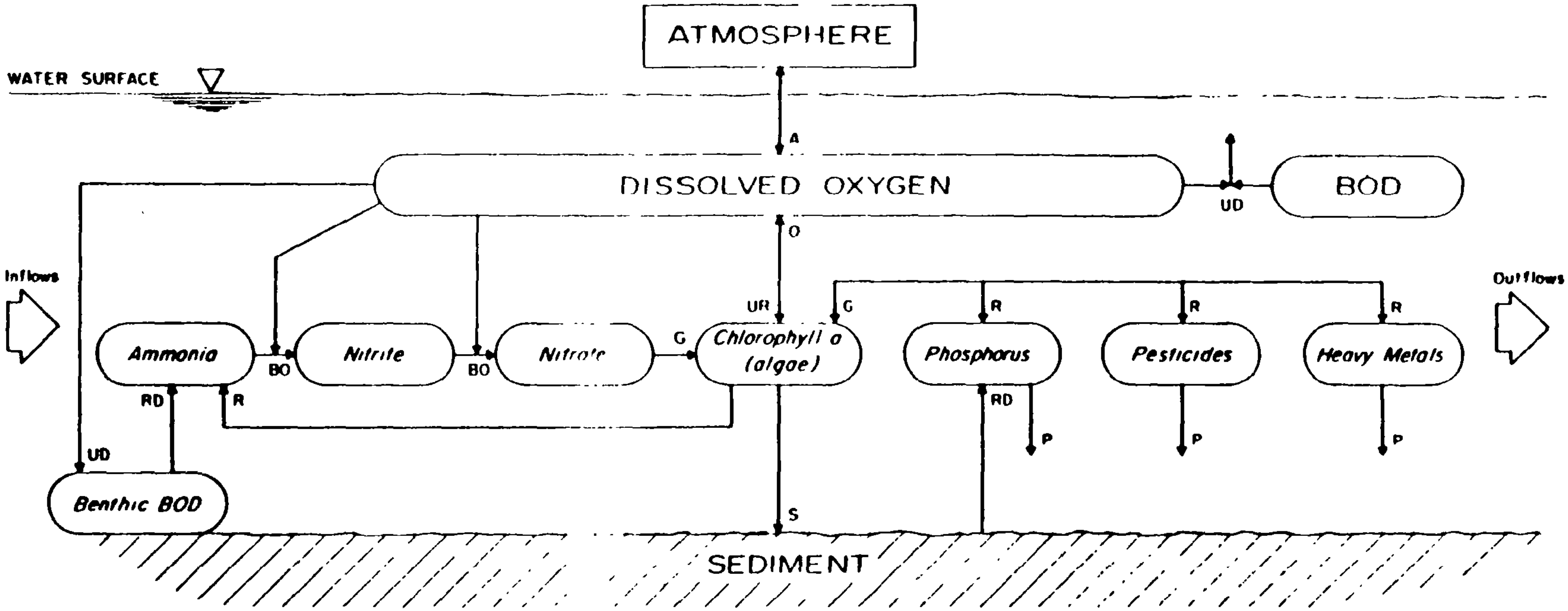
where

P = orthophosphate concentration,
K_p = empirical half saturation constant for nitrogen.

III.2.8 DISSOLVED OXYGEN

A simplistic approach to the analysis of dissolved oxygen (DO) concentrations would be to consider the DO reaeration process at the water surface and the DO uptake from the BOD decay. If this approach is used, then the reaeration rate and BOD decay rate are actually representing all the other water quality actions and reactions which may be adding to or depleting the supply of DO in the estuary. If the nitrogen cycle is considered, then in addition to the BOD uptake, the oxidation of ammonia to nitrite, and nitrite to nitrate will deplete the supply of oxygen. For those cases where sludge deposits or other sédiment conditions which exert an oxygen demand on the water column above the sediment bed, a benthic oxygen demand can be included in the processes to describe the dissolved oxygen concentration. Where algal biomass is considered in the water quality processes of the estuary, DO is supplied to the system during algal growth and DO is taken from the system during algal respiration.

The change in dissolved oxygen concentration, as discussed above, is a function of many other water quality parameters. Figure III-3 demonstrates graphically the interrelationship and mechanisms of change formulated as part of one water quality model, the Dynamic Estuary Model (Genet, et al., 1974). This diagram which shows the relationships of BOD, nitrogen, and algae to dissolved oxygen, also displays the models mechanism of change for phosphorus, pesticides, and heavy metals.



A	AERATION - DEAERATION	R	RESOLUBILIZED DURING RESPIRATION
BO	BIOCHEMICAL OXIDATION	RD	RESOLUBILIZED WITH DECAY
G	CONSUMED DURING ALGAL GROWTH	S	REMOVED BY SETTLING
O	OXYGENATION DURING ALGAL GROWTH	UD	UPTAKE WITH DECAY
P	PRECIPITATION	UR	UPTAKE WITH RESPIRATION

Figure III-3. Interrelationships and Mechanisms of Change in the Dynamic Estuary Model (Genet et al, 1974).

Many actions and reactions of water quality constituents increase or decrease the dissolved oxygen concentration in the water body. The rate of change of dissolved oxygen can be described in the following form:

$$\frac{dO}{dt} = K_2(O^*-O) + (k_1 g_a - k_2 r_a)A - K_1(BOD)$$

$$- \frac{K_{17}}{d} - k_3 K_{11}(NH3) - k_4 K_{13}(NO2) \qquad \text{(III-16)}$$

where

O = dissolved oxygen concentration,

O^* = saturation concentration of dissolved oxygen at the local temperature, pressure and chloride concentration,

K_2 = reaeration rate,

k_1 = rate of oxygen production per unit of algae during photosynthesis,

g_a = specific growth rate of algae,

k_2 = rate of oxygen uptake per unit of algae respired

r_a = respiration rate of algae,

A = concentration of algae,

K_1 = rate of decay of carbonaceous BOD,

BOD = carbonaceous biochemical oxygen demand,

K_{17} = benthic oxygen demand,

d = depth,

k_3 = rate of oxygen uptake per unit of ammonia oxidation,

K_{11} = rate of biological oxidation of ammonia,

NH3 = ammonia concentration,

k_4 = rate of oxygen uptake per unit of nitrite oxidation,

K_{13} = rate of oxidation of nitrite,

NO2 = nitrite concentration.

III.2.9 TOXICANTS

The transport and transformations (i.e., the fate) of toxic substances can be very complex. However, many heavy metals are considered as conservatives and organic chemicals are considered to decay using first order kinetics. Toxic substances are not only transported and transformed in the water column, but bottom sediment is also a transport medium for toxicants which can remain in the sediment for years.

Unlike many conventional pollutants, such as BOD, toxic substances are not necessarily transformed into harmless substances. In some cases, they are tranformed into equally toxic substances or into a substance which is more toxic than the original substance. The primary transformation processes include photolysis, hydrolysis, and biodegradation.

Photolysis

Photolysis is the process in which the absorbtion of light causes chemical decomposition of the toxicant. There are two general types of photolysis; direct and sensitized (Tetra Tech, 1982). Direct photolysis occurs when the toxic substance reacts to direct light which it has absorbed. Sensitized photolysis, or photosensitization, occurs when a molecule which has absorbed light transfers its excess energy to another molecule which absorbs the energy. The overall rate of photolysis is the sum of the two types. The reaction kinetics can be expressed as a first order decay as follows:

$$\frac{dC}{dt} = - K_p C \qquad \text{(III-17)}$$

where

C = toxicant concentration,
K_p = sum of photolysis rates,

$$= Kd + Ks$$

where

Kd = direct rate,
Ks = sensitized rate.

Hydrolysis

The toxicant may also react chemically with the H^+ and OH^- ions of water to form a weaker substance. This process is known as hydrolysis. Hydrolysis can occur by microbial meditated reactions or abiotic reactions (Tetra Tech, 1982). The microbial actions become part of the process of biodegradation as discussed below. Abiotic hydrolysis can be expressed as a first order decay as follows:

$$\frac{dC}{dt} = - K_H C \tag{III-18}$$

where

C = concentration of toxicant,
K_H = specific hydrolysis rate constant.

Biodegradation

Many toxic substances are transformed by microbial organisms. In this process of biodegradation, the organisms metabolize the substance and change its form and level of toxicity. There are two metabolic patterns in the process of biodegradation (Tetra Tech, 1982). The first, growth metabolism, occurs when an organic toxicant is used as a food source by the microorganism. The second, called cometabolism, occurs when the organic toxicant is transformed by the microorganism but the organism does not derive any benefit for growth from the reaction. These two processes have different rates of degradation.

For growth metabolism, first order decay can be applied to describe the kinetics in the aquatic environment. The formula is:

$$\frac{dC}{dt} = - K_B C \qquad \text{(III-19)}$$

where

C = concentration of toxicant,
K_B = biodegradation rate constant.

For cometabolism, the rate is directly proportional to the size of the microbial population. The process can be represented as a second order law as follows:

$$\frac{dC}{dt} = - K_{B2}(B)(C) \qquad \text{(III-20)}$$

where

C = concentration of toxicant,
K_{B2} = second-order biodegradation rate,
B = bacterial population.

III.2.10 AQUATIC ECOSYSTEM

In addition to the processes discussed above, other processes of an ecosystem can affect and be affected by the water quality in an estuary. A conceptual model of an aquatic ecosystem is given in Figure III-4 (Chen and Orlob, 1971).

An aquatic ecosystem is comprised of water, its chemicals and various life forms: bacteria, algae, zooplankton, benthos, and fish, among others. Biota respond to nutrient availability and to other environmental conditions that affect growth, respiration, decay, mortality, and predation. Abiotic substances, derived from air, soil, tributary waters and the

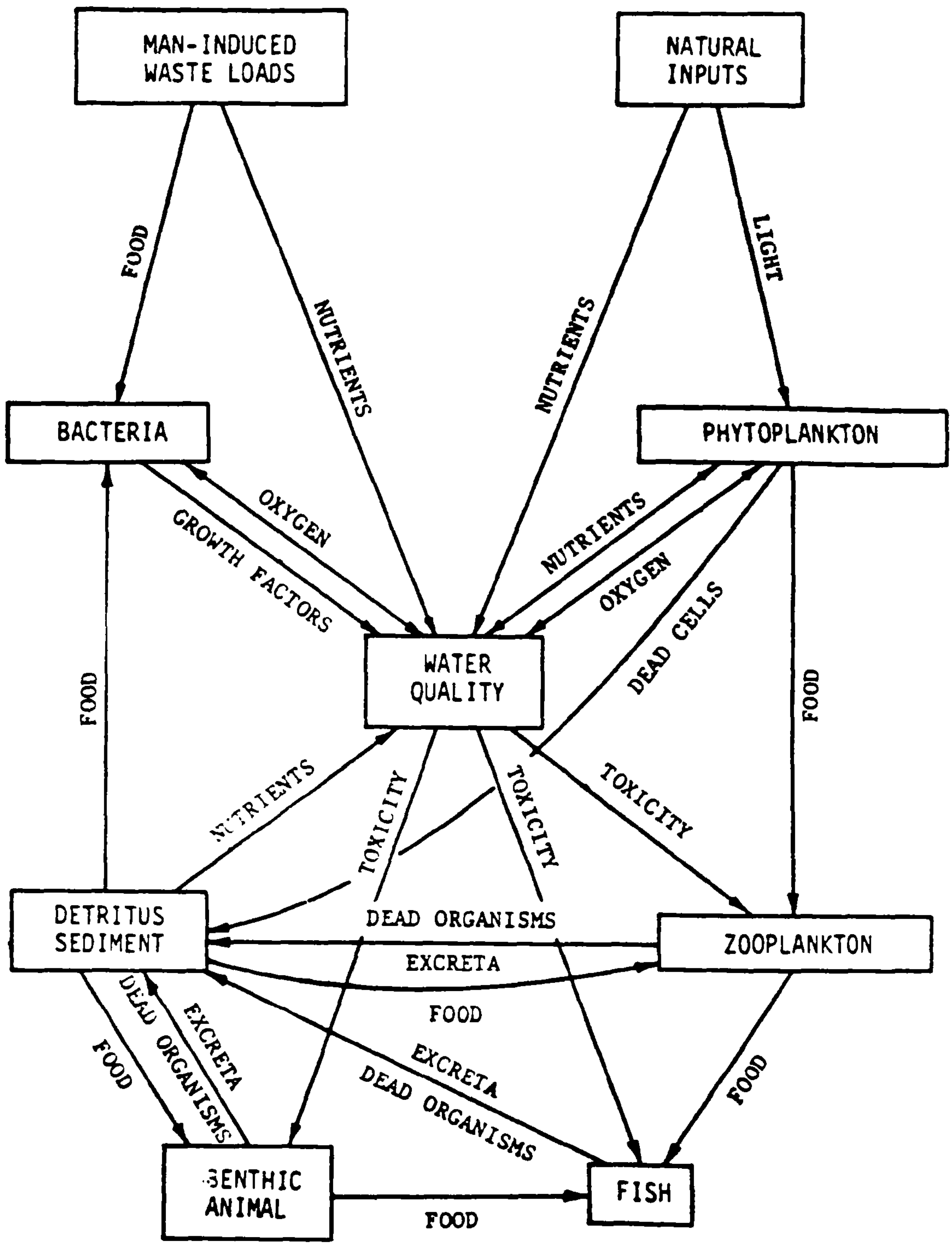


Figure III-4. Conceptual Model of an Aquatic Ecosystem (Chen and Orlob, 1977) activities of man, are inputs to the system that exert an influence on the estuary life structure.

The fundamental building blocks for all living organisms are nutrients. With solar radiation as the energy source, these inorganic nutrients are transformed into complex organic materials by photosynthetic organisms. The organic products of photosynthesis serve as food sources for aquatic animals. It is evident that a natural succession up the food chain occurs whereby inorganic nutrients are transformed to biomass and ultimately are passed to man.

Biological activities generate wastes, consisting of respired nutrients, dead cell material and excrete, which initially are suspended but settle to the bottom to become organic sediments. Detritus and organic bottom sediments decay with the attendant release of the original abiotic substances. These transformations include the nitrogen and phosphorus cycles and result in a natural "recycling" of nutrients within an aquatic ecosystem.

Specific processes not discussed in the previous sections are presented below:

Zooplankton

Zooplankton feed on the phytoplankton (algae) depending on the abundance of the algae and the zooplankton's preference for various types of algae. The concentrations of zooplankton depend on their growth rate, mortality rate, respiration rate and fish predation.

Benthic Animals

Benthic animals use organic sediment as a food source and are grazed by fish. The benthic animal density is a function of the benthos growth, mortality and respiration rates, and fish predation.

Fish

Fish growth, respiration and mortality are a function of the dissolved oxygen concentration and food availability. Fish are typically divided into herbivores and carnivores. Herbivores feed principally on living plants, while carnivores feed principally on animals that they kill. Another type, omnivore, feeds on plants and animals alike. Fish populations can be reduced by the top-carnivores and by fish harvest by man.

Detritus

Detritus consists of dead zooplankton and suspended excreta derived from zooplankton and fish. Detritus is removed from the system by sedimentation and decay.

Organic Sediment

Organic sediment is the food source for benthic animals and is composed of dead biota. Algae and detritus are converted to organic sediment when they settle to the estuary bottom. Sediment decay serves both as a dissolved oxygen sink and a source of inorganic nutrients.

III.3 REACTION RATES AND CONSTANTS

The chemical and biological reactions that occur in the biochemical processes are dependent on various reaction rates and physical constants. Some of these coefficients are constant and some are temperature dependent. Table III-1 lists several of the more commonly used conventional parameters, gives the units and possible ranges of the reaction rates for each parameter. Care must be taken in applying these coefficients. Some are highly variable and the values and units of others are dependent on the particular formulation in a given estuary model. A more extensive literature review of rate parameters used in surface water quality models can be found in "Rates, Constants, and Kinetics Formulations in Surface Water Quality Modeling" (Zison, et al., 1978).

TABLE III-1

REACTION RATES AND CONSTANTS FOR CONVENTIONAL POLLUTANTS

DESCRIPTION	UNITS	RANGE OF VALUES	TEMPERATURE DEPENDENT	RELIABILITY
Fraction of algae biomass which is N	$\frac{mg\ N}{mg\ A}$	0.07-0.09	No	Good
Fraction of algae biomass which is P	$\frac{mg\ P}{mg\ A}$	0.012-0.015	No	Good
O_2 production per unit of algae growth	$\frac{mg\ O}{mg\ A}$	1.4-1.8	No	Good
O_2 production per unit of algae respired	$\frac{mg\ O}{mg\ A}$	1.6-2.3	No	Fair
O_2 uptake per unit of NH_3 oxidation	$\frac{mg\ O}{mg\ N}$	3.0-4.0	No	Good
O_2 uptake per unit of NO_2 oxidation	$\frac{mg\ O}{mg\ N}$	1.0-1.5	No	Good
Maximum specific growth rate of algae	$\frac{1}{day}$	1.0-6.0	Yes	Good
Algae respiration rate	$\frac{1}{day}$	0.01-0.5	Yes	Fair
Rate constant for biological oxidation of NH_3-NO_2	$\frac{1}{day}$	0.05-0.5	Yes	Fair
Rate constant for biological oxidation of NO_2-NO_3	$\frac{1}{day}$	0.5-2.0	Yes	Fair
Local settling rate for algae	$\frac{ft}{day}$	0.5-6.0	No	Fair
Carbonaceous BOD decay rate	$\frac{1}{day}$	0.05-2.0	Yes	Poor
Reaeration rate	$\frac{1}{day}$	0.0-100	Yes	Good
Coliform die-off rate	$\frac{1}{day}$	0.5-4.0	Yes	Fair
Nitrogen half-saturation constant for algae growth	$\frac{mg}{l}$	0.1-0.4	No	Fair to Good
Phosphorus half-saturation constant for algae growth	$\frac{mg}{l}$	0.03-0.05	No	Fair to Good
Light half-saturation constant for algae growth	$Kcal/m^2/sec$	0.002-0.006	No	Good

Toxicant reaction rates are highly variable and depend on the particular pollutant under consideration, and on the transformation process or processes being simulated by the model. For example, if for a particular toxicant the abiotic hydrolysis rate is 20 times faster than the biodegradation rate, then the simulation of the transformation can neglect the biodegradation process without significantly impacting the model result. A good source of reaction rates for a wide range of compounds for biodegradation, near-surface direct photolysis and hydrolysis is available in "Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants - Part 1 (Mills, et al., 1982).

The references cited for information on reaction rates (Zison, et al., 1978; and Mills, et al., 1982) provide a basic starting point for selecting various reaction rates and constant. Documentations and users manuals for estuary models may also contain ranges of the reaction rates applied in the particular model. The final selection of the values for many of the reaction rates and constant should be made during model calibration and verification.

III.3.1 REAERATION RATE

It is important to obtain good estimates of all the reaction rates. Many initial estimates of the rates can be obtained from the analysis of field and laboratory water quality data. In most model formulations the reaction rates are input directly into the model.

In this section additional discussion is provided concerning the reaeration rate because it is highly dependent on the hydrodynamic properties of the estuary, and some models include formulas which calculate the K_2 rate. There have been a variety of studies which have produced equations for determining the reaeration rate. Many of them rely on the velocity and depth to calculate the reaeration coefficient. Most of these formulations have been developed from river and stream studies, and they may not be applicable to estuary studies. Zison, et al. (1978) relate that for modeling non-stratified estuaries, the equation by O'Connor (1960) has probably been the most widely used formulation which contains velocity and depth. O'Connor's expression is:

$$K_2 = \frac{(D_m U_o)^{0.5}}{H^{1.5}} \tag{III-21}$$

where

K_2 = reaeration rate,
D_m = molecular diffusivity of oxygen,
U_o = mean tidal velocity over a complete tidal cycle,
H = average depth at a section over the tidal cycle,

and any consistent units are used.

Several estuary models include this formulation. However, models also allow for user input of the reaeration coefficients. Therefore, like all other reaction rates, the final K_2 rate will be determined during the process of model calibration and verification.

III.3.2 TEMPERATURE DEPENDENCE

All reaction rate constants and some other factors (except the saturation concentration of oxygen) that are known to be temperature dependent are usually formulated by applying an exponential temperature adjustment factor to the reaction rate at 20°C. The equation is:

$$K_T = K_{20}\, \theta^{(T-20)} \tag{III-22}$$

where

K_T = reaction rate at temperature T,
T = ambient temperature of water body in °C,
K_{20} = reaction rate at 20°C,
θ = empirical constant for a given reaction rate.

The temperature adjustment factor, θ, varies for different reaction rates. Different investigators have used different adjustment factors for the same reaction rate. Values of the temperature adjustment factors are presented by Zison, et al. (1978).

III.4 TIME AND SPACE SCALES

The time and space scales as they relate to water quality processes depend on the problem being addressed. Time scales relate to the time cycle being simulated and the duration of the total simulation. Space scales relate to the longitudinal, lateral, and vertical definitions required.

III.4.1 TIME SCALES

The major temporal dimensions are those considered by steady state, tidally averaged and real time models. The selection of a time scale will depend on, for example, whether the problem is to predict the summer chlorophyll-a concentration from the spring load of nutrients or the diurnal dissolved oxygen variation as a function of algae photosynthesis and respiration.

Real time models which simulate the tidal cycle are appropriately used for analyzing changes which occur within a tidal cycle. These models can simulate the estuary response over short durations of nonpoint source loads from a storm event and point source spills. Whenever it is desirable to simulate the concentration and location of a waste plume, in a tidal estuary, a real time model must be used. Where minimum or maximum water quality criteria are given at any time in addition to a daily average value, then a real time model can simulate the variations over the tidal cycle and predict the minimum or maximum constituent concentration that occurred during the day.

If diurnal variations are important to the wasteload allocation study, then real time models must be used. They can be used to predict the diurnal dissolved oxygen variation as a function of algal photosynthesis and respiration.

Figure III-5 illustrates a typical pattern of diurnal DO response. The primary points of interest on this curve are the points labeled A and B. The value of the dissolved oxygen at point A is taken to represent the "average" DO concentration, ignoring the diurnal effects produced by plant communities. The dissolved oxygen deficit, C-A, represents the deficit caused by BOD exertion. The DO at point B is the minimum DO for the day. The dissolved oxygen deficit at this point, C-D, represents the net total community respiration on the stream oxygen resources. The magnitude of the deficit, A-D, can be considered to represent the maximum deficit over the daily cycle attributable to aquatic plant respiration.

Steady state or tidally averaged models cannot predict the water quality variation over a tidal cycle. They are useful in predicting larger term (daily or seasonal) effects of the actions and interactions of the water quality constituents. For example, they can be used to predict the growth of algal blooms which may take several days.

It is also important to consider the total duration of the model simulation for temporal dimensions other than steady state. The model must simulate a long enough period of time so that the water quality parameters have had enough time to react and reach their minimum or maximum values. A large oxygen consuming load from a localized storm event in one part of the estuary watershed may take several days to produce the minimum dissolved oxygen concentration in another, downstream, part of the estuary. The simulation period must be long enough to show the beginning of the dissolved oxygen recovery in order to demonstrate that the minimum dissolved oxygen sag value has occurred. As another example, consider the simulation of fecal coliform die-off from a storm or point source by-pass. If the investigator is interested in the time when 90 percent of the coliform population has died-off (T_{90}), then the duration of the simulation may have to be half a day or several days, depending on the die-off rate used.

In the above discussions of biochemical processes, reaction kinetics were frequently described by a decay rate or reaction rate, K. This can be

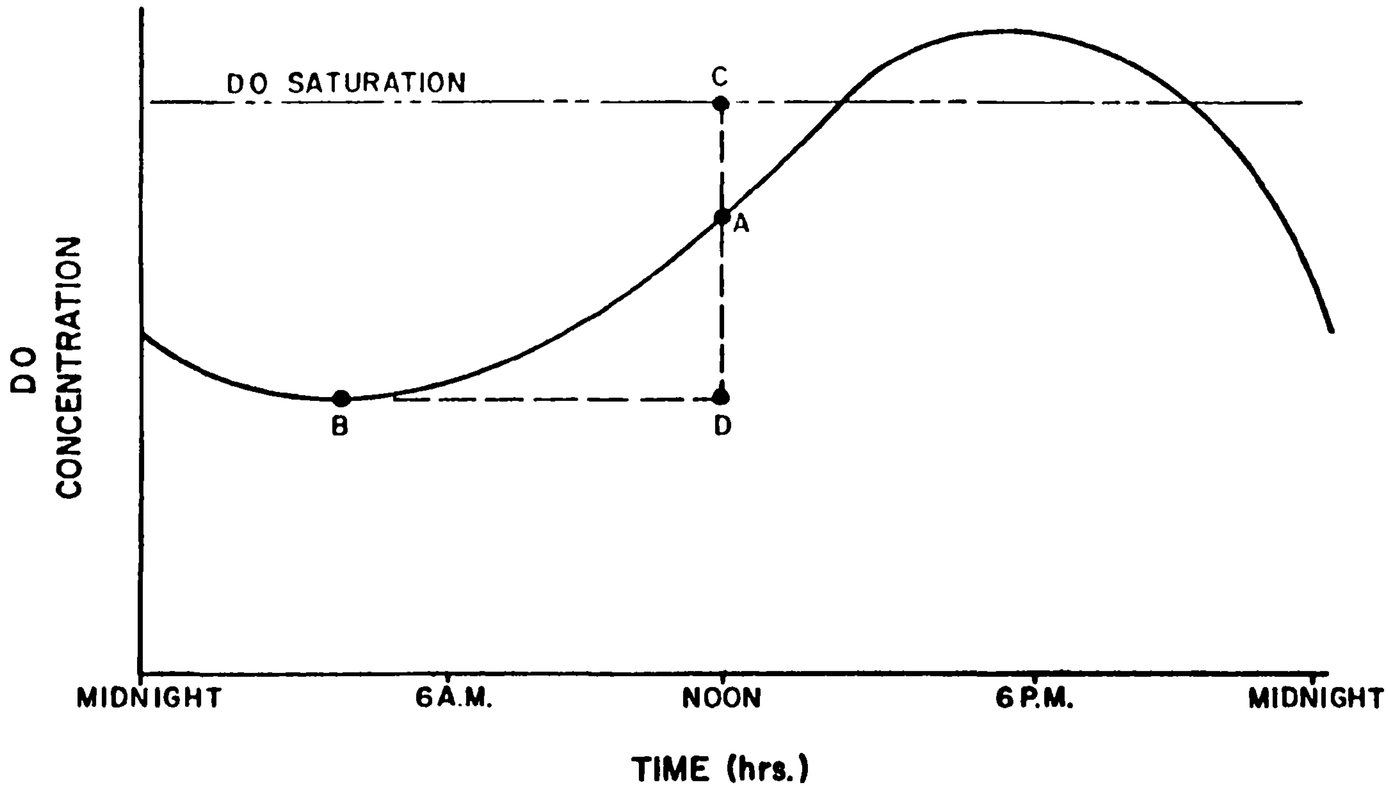


Figure III-5. Diurnal Dissolved Oxygen Variation converted to a process rate time scale characterized by the time to achieve 90 percent reduction, T_{90}, by:

$$T_{90} = 2.3/K \qquad \text{(III-23)}$$

This biochemical time scale can then be compared with physical time scales to select appropriate processes.

III.4.2 SPACE SCALES

Space scales are determined to adequately model the longitudinal, lateral and vertical dimensions. Models are usually developed along the horizontal with various segments or in a node-link manner. The longitudinal distance between nodes or segments where water quality calculations are made must be spaced so that they will adequately simulate the spatial variability in the water quality and biological communities. The distance must be small enough to simulate the actual maximum or minimum constituent concentrations of concern. For example, if under certain conditions the dissolved oxygen sag occurs a distance of 2 km from the point of discharge, then the distance between water quality computations cannot be greater than 2 km or the model would inaccurately locate the point of minimum dissolved oxygen.

In addition to defining the proper longitudinal scale for water quality computational purposes, it is important to design the length of the segments or links in order to adequately receive important point and nonpoint sources of pollution as input to the model. This is not usually a problem if variable length segments or links can be accommodated by the model.

For a very wide estuary or wide segments of an estuary, it may be important to show the lateral variations of water quality constituent, thus requiring a two-dimensional network. Concentration will vary laterally in a wide estuary especially near the major points of discharge where the pollution load has not been completely mixed across the estuary. It is possible that a stream standard could be violated on one side of the estuary but not on the other side. The physical properties such as depth and velocity may also vary laterally across the estuary. This can affect the prediction of the reaeration rates which are a function of velocity and depth, and thereby affect the dissolved oxygen prediction.

Vertical space scales can also be important in those estuaries which stratify, that is, where a large density gradient exists between the upper freshwater and the lower saltwater region of an estuary. At the depth of the greatest gradient difference (pycnocline), transfer of water quality constituents from the freshwater layer to the saltwater layer and vice versa is inhibited. One major factor in this phenomenon is the variability of the dissolved oxygen on the vertical scale. The reaerated surface waters cannot mix with the bottom waters and, therefore, the dissolved oxygen concentrations in bottom waters becomes depleted by the oxygen consuming constituents and benthos. Major changes can occur in the aquatic ecosystem if the dissolved oxygen concentrations approach or go to zero in the bottom waters. Models which can formulate networks with vertical slices or levels instead of a system which is completely mixed vertically can be applied for those estuaries which are highly stratified.

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SECTION IV

FRAMEWORK FOR MODEL SELECTION

The approach to numerical model selection in the past has been essentially intuitive, with a tendency to ush one's own model rather than choose the best model to do the job. In this section, we will lay out a stepwise framework which can be used as a basis for model selection.

The rationale behind the framework is to identify and evaluate the importance of physical/chemical/biological characteristics of the study area and to define a set of objectives for the study. The method of selecting an appropriate model is then to identify the set of available models that can simulate the important processes within the time and spatial scales of the study. These scales define bounds with which the study is performed. These scales are then divided into time and space intervals which provide resolution within the study bounds.

The proposed framework has eleven steps (see Figure IV-1):

1. Develop a conceptual model;
2. Develop a definition of complete mixing;
3. Define far-field dimensions which cannot be reduced;
4. Determine time and spatial scales of processes and constituents;
5. Determine time and spatial scales of regulations;
6. Determine which spatial scales can be neglected at the study scale;
7. Determine whether a fully dynamic model is needed;
8. Determine desired spatial and temporal resolution;
9. Select form of the dispersion coefficient;
10. Check data availability; and
11. Select appropriate model(s).

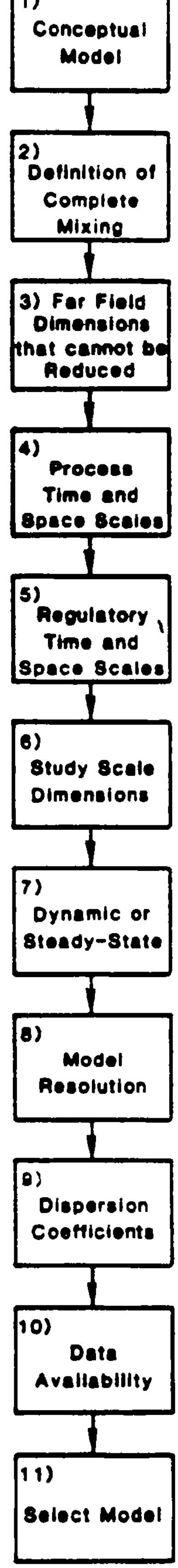


Figure IV-1 FRAMEWORK FOR MODEL SELECTION

IV.1 CONCEPTUAL MODEL

A useful starting point for numerical model selection is to conceptualize the system being studied. This can be done either as a set of equations describing the various physical/chemical/biological processes, a written description of them, or perhaps, most usefully, a schematic representation of them. The figure is perhaps the most useful form, as one can readily visualize the system's processes. The schematic representation can be in the form of a diagram of the system and its processes (Figure IV-2) or else in the form of relationship charts of parts of the system (Figure IV-3).

The purpose of this step is to assimilate and present all the available knowledge of a system in a way that major processes and ecologic relationships can be evaluate for inclusion in the numerical model description. The conceptual model is the starting point from which systematic reductions in complexity can be made which will provide an adequate representation of the system, while meeting the objectives of the study.

IV.2 DEFINITION OF COMPLETE MIXING

Complete mixing in a numerical model is a theoretical concept only. This is because given any model with spatial resolution, dispersion is treated as a gradient process. Only in the limit as t can complete mixing be achieved numerically. It thus becomes necessary, in a practical sense, to develp some definition of complete mixing over a spatial dimension that provides an acceptable point at which uniformity in that spatial dimension can be assumed and that dimension neglected. For example, if we wish to use a one-dimensional, cross-sectionally averaged, mass transport model, the assumption is implicitly made that actual concentration deviations from the cross-sectional mean are acceptable within an error tolerance.

There are several way in which a definition might be established over the dimension being analyzed. Consider the definition sketch of an actual distribution over the lateral dimension, y, shown in Figure IV-4. One definition might be:

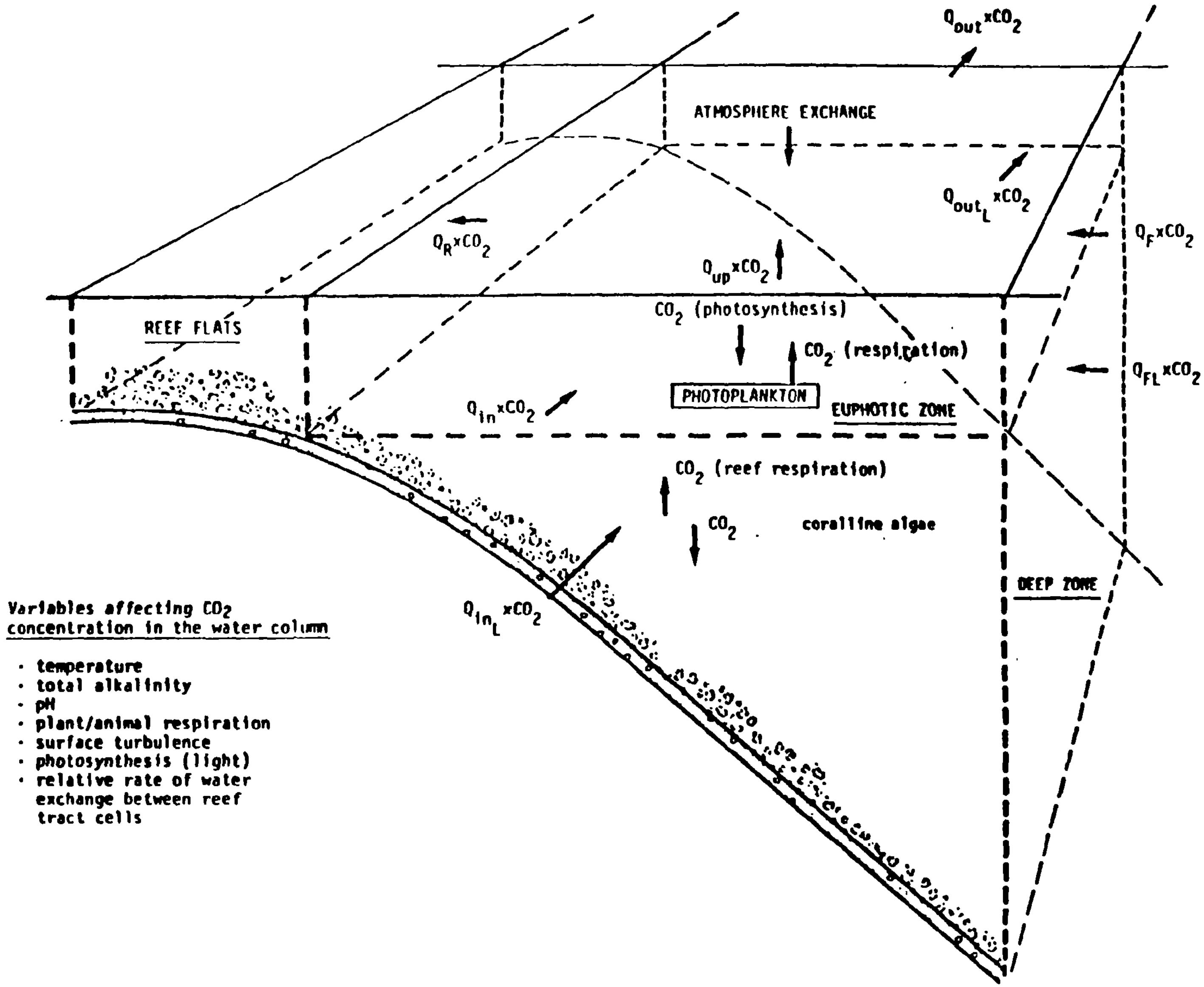


Figure IV-2. Representation of CO_2 Mass Balance in Reef Tract.

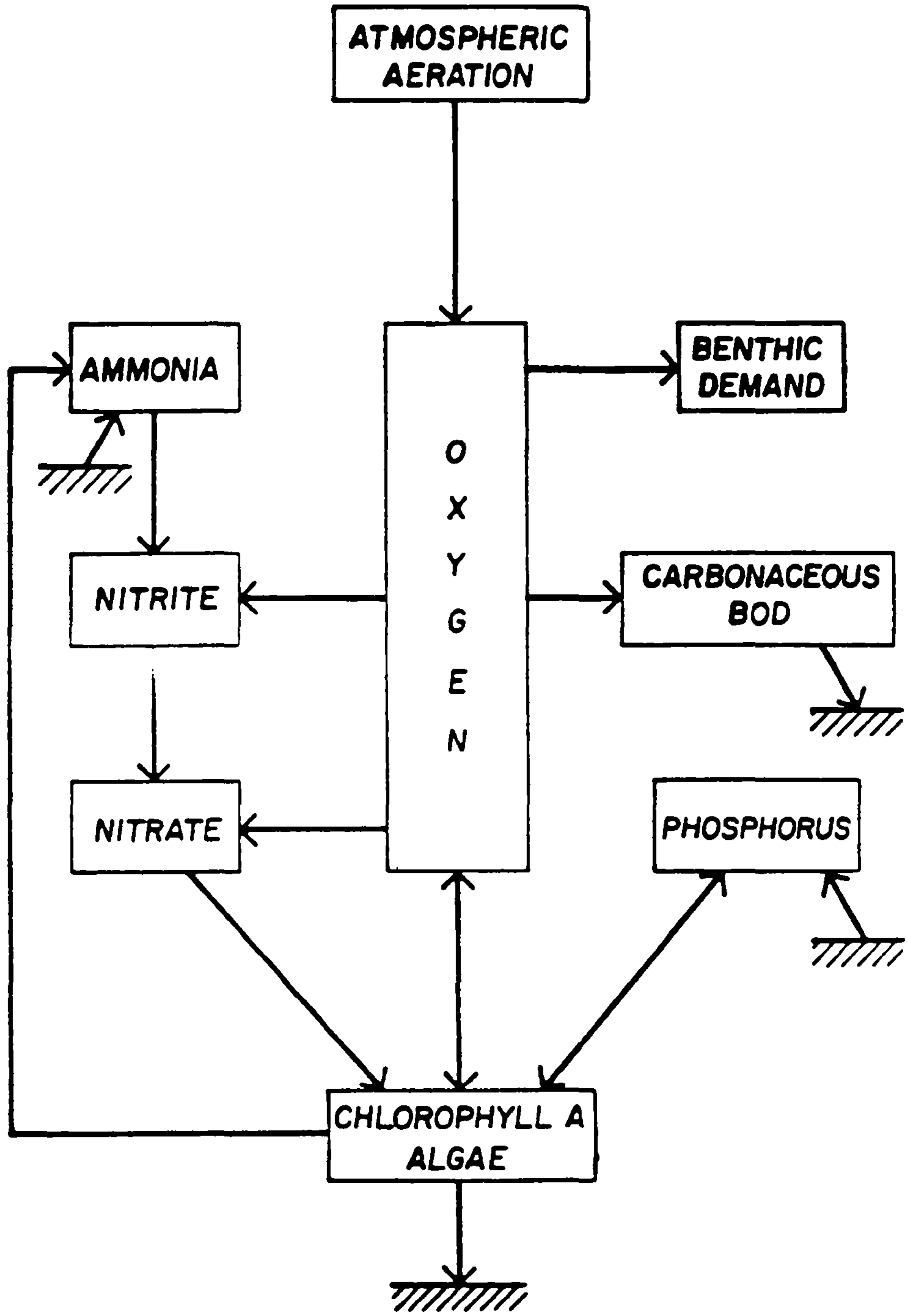


Figure IV-3 Major Constituent Interactions

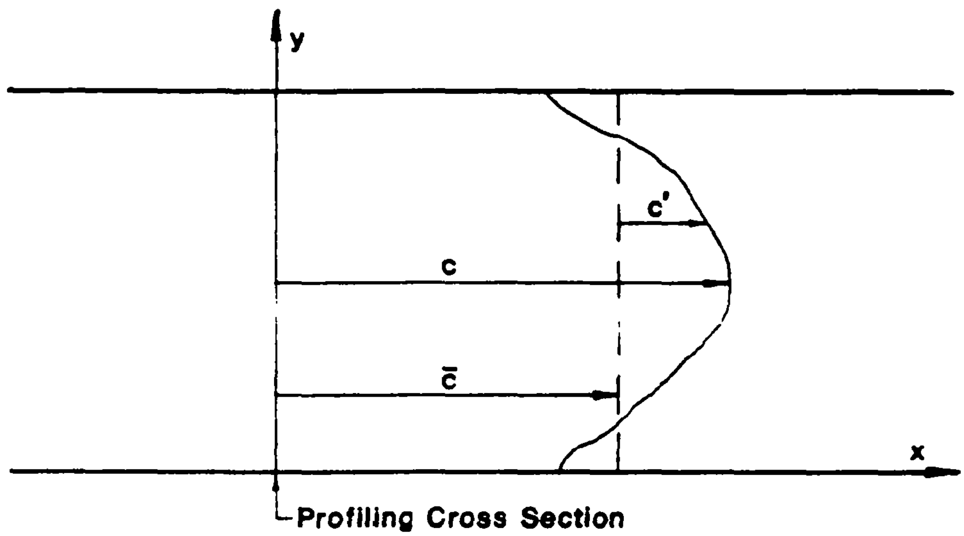


Figure IV-4 LATERAL CONCENTRATION DISTRIBUTION

$$|c'_{max}| / \bar{c} \quad < \quad T_1 \qquad \text{(IV-1)}$$

where c'_{max} = maximum concentration deviation

$\bar{c}$ = average concentration over dimension, y, and

T_1 = acceptable error tolerance.

A second definition might be:

$$c_{max} / \bar{c} \quad < \quad T_2 \qquad \text{(IV-2)}$$

where c_{max} = maximum concentration value, and

T_2 = acceptable error tolerance.

The crux of the problem is to assign suitable values to T_1 or T_2. Factors involved in choosing these values are errors in field measurements, errors in simulated values, and acceptable deviation from the mean value, $\bar{c}$.

IV.3 FAR FIELD DIMENSION REDUCTION

It is usually practical to choose a numerical model with as simple a description of the prototype physical/chemical/biological processes as will yield sufficiently accurate results. A common approach to simplifying the analysis is to neglect one or more spatial dimensions (usually the vertical and/or lateral) over which the constituent being modeled can be assumed to be completely well-mixed from the definition developed. Reductions in dimensionality, when justifiable, can realize considerable savings in model development/modification and simulation costs. As a first step to reducing dimensionality, one can consider the inverse condition - which dimensions cannot be neglected in the far field (at distances a long way away from the point(s) of discharge(s)). Considerations here include whether the system is stratified, in which case the vertical dimension must be included, whether flow reversal are observed, etc. This step is often straightforward, and simplifies later analysis in which finer-scale fields are analyzed because it will limit such analyses to those dimensions over which the system might be considered to be well mixed.

For estuarine modeling, we will assume that the longitudinal (x) dimension cannot be neglected (as is sometimes the case for reservoir modeling). The objective of this step, then, is to evaluate whether the lateral (y) or vertical (z) dimensions must be retained.

IV.3.1 VERTICAL DIMENSION

The most frequent cause of variations in the vertical direction is density stratification. This can be observed in one of several ways:

- o salinity and/or temperature gradients,
- o tidal or residual velocity reversals,
- o dye cloud splitting and differential advection, and/or
- o geomorphological classification.

Degree of Stratification.

Freshwater is lighter than saltwater. This produces a buoyance of amount:

$$\text{Buoyancy} = \Delta\rho\, g\, Q_R \tag{IV-3}$$

where $\Delta\rho$ = the difference in density between sea and river water, (M/L^3)
g = acceleration of gravity, (L/T^2), and
Q_R = freshwater river flow, (L^3/T)

The tide on the other hand is a source of kinetic energy, equal to:

$$\text{kinetic energy} = WU_t^{\,3} \tag{IV-4}$$

where ρ = the seawater density,
W = the estuary width
U_t = the square root of the averaged squared velocities.

The ratio of the above two quantities, called the "Estuarine Richardson Number" (Fischer, 1972), is an estuary characterization parameter which is indicative of the vertical mixing potential of the estuary:

$$R = \frac{\Delta\rho\ g\ Q_R}{\rho\ W U_t{}^3} \qquad \text{(IV-5)}$$

If R is very large (above 0.8), the estuary is typically considered to be strongly stratified and the flow dominated by density currents. If R is very small, the estuary is typically considered to be well-mixed and the density effects to be negligible.

Another desktop approach to characterizing the degree of stratification in the estuary is to use a stratification-circulation diagram (Hansen and Rattray, 1966). The diagram (shown in Figure IV-5) requires the calculation of two parameters:

$$\text{Stratification Parameter} = \frac{\Delta S}{S_o} \qquad \text{(IV-6)}$$

$$\text{and Circulation Parameter} = \frac{U_s}{U_f}$$

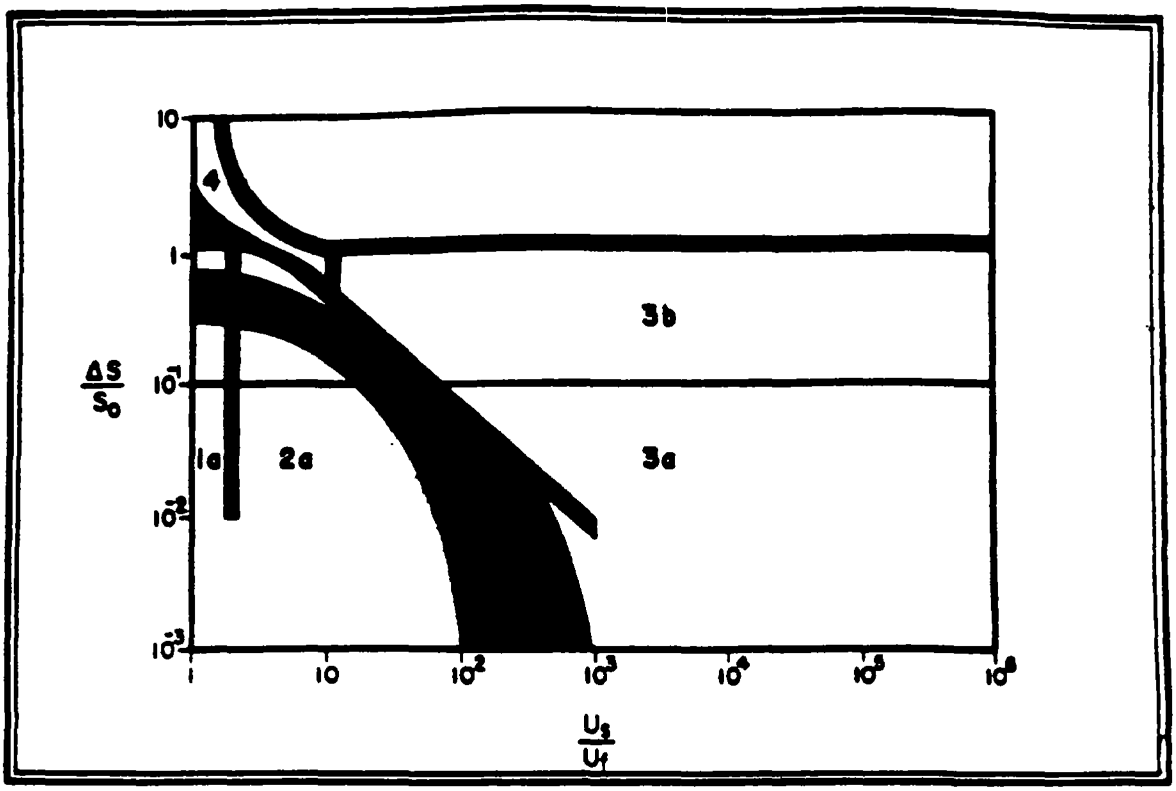
where ΔS = time averaged difference between salinity levels at the surface and bottom of the estuary,

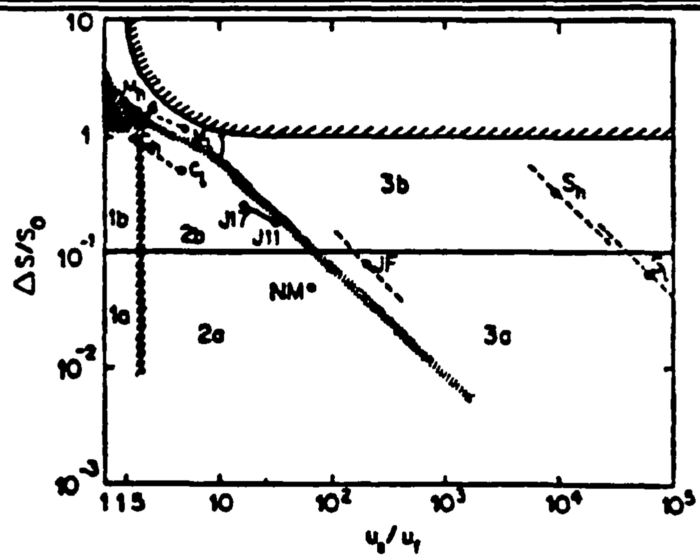
S_o = cross-sectional mean salinity,

U_s = net non-tidal surface velocity, and

U_f = mean freshwater velocity through the section.

To apply the stratification-circulation diagram in Figure IV-5, which is based on measurements from a number of estuaries with known degrees of stratification, calculate the parameters of Equation (IV-6) and plot the resulting point on the diagram. Type 1a represents slight stratification as in a laterally homogeneous, well-mixed estuary. In Type 1b, there is strong stratification. Type 2 is partially well-mixed and shows flow reversals with depth. In Type 3a the transfer is primarily advective, and in Type 3b the lower layer is so deep, as in a fjord, that circulation does not extend to the bottom. Finally, Type 4 represents the salt-wedge type with intense stratification (Dyer, 1973).





(Station code: M, Mississippi River mouth; C, Columbia River estuary; J, James River estuary; NM, Narrows of the Mersey estuary; JF, Strait of Juan de Fuca; S, Silver Bay. Subscripts h and l refer to high and low river discharge; numbers indicate distance (in miles) from mouth of the James River estuary.

Figure IV-5. Stratification Circulation Diagram and Examples.

The purpose of the analysis is to examine the degree of vertical resolution needed for the analysis. If the estuary is well-mixed, the vertical dimension may be neglected, and all constituents in the water column assumed to be dispersed evenly throughout. If the estuary is highly stratified, at least a 2-layer analysis must be used. For the case of a partially-mixed system, a judgment call must be made. The James River may be considered as an example which is partially stratified but was treated as a 2-layer system for a recent toxics study (O'Connor et al., 1983).

A final desktop method for characterizing the degree of stratification is the calculation of the estuary number proposed by Thatcher and Harleman (1972):

$$E_d = \frac{P_t F_d^2}{Q_f T} \qquad \text{(IV-7)}$$

where E_d = estuary number,
P_t = tidal prism volume, (L^3)
F_d = densimetric Froude number,
Q_f = freshwater inflow, (L^3/T), and
T = tidal period, (T).

Again, by comparing the calculated value with the values from known systems, one can infer the degree of stratification present.

Once the degree of stratification is determined by one of the above methods, we recommend the following criteria:

strongly stratified	- include the vertical dimension in at least a 2-layer model
moderately stratified	- include the vertical dimension in a multi-layered model, or reserve judgment to the calculations in Step 6, and
vertically well-mixed	- could neglect vertical dimension after calculation in Step 6.

Tidal or Residual Velocity Reversals

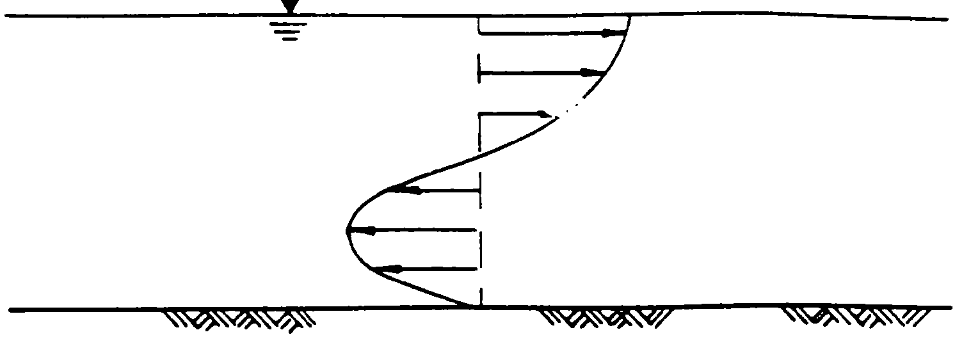
Beyond the use of a stratification diagram, the analysis of vertical dimension reduction becomes more difficult and intuitive. However, the following criteria seem reasonable (Figure IV-6):

tidal velocity reversals	- include vertical dimension in at least a 2-layer model,
residual velocity reversals	- include the vertical dimension in a multi-layered model or reserve judgment to the calculation in Step 6, and
no observable reversals	- could neglect vertical dimension after calculation in Step 6.

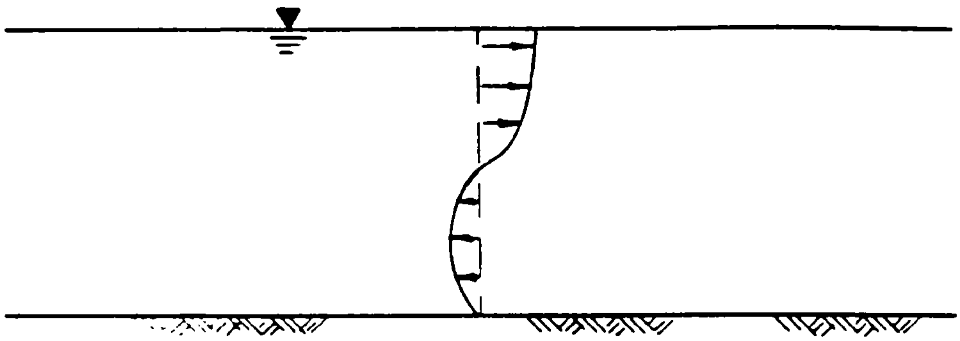
Dye Studies

Dye studies simply replace the Eulerean observations of current meters with the Lagrangian movement of a dye cloud study. Again, quantitative analyses are difficult, but the following criteria seem reasonable (Figure IV-7):

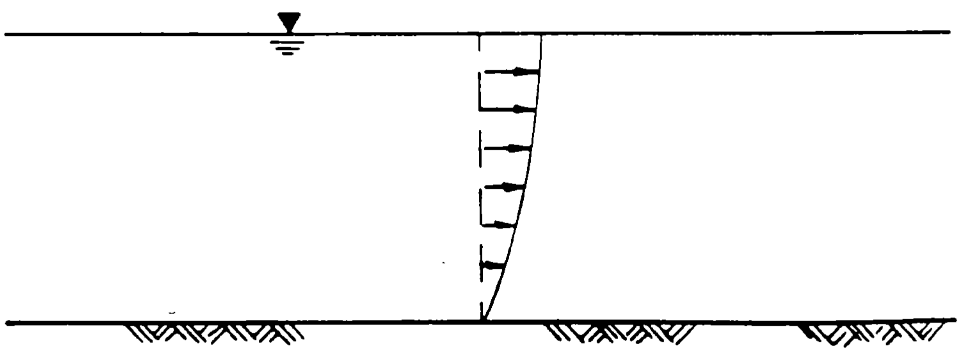
Dye cloud separates and moves	- cloud is responding to a vertical flow reversal and moves as 2 or more distinct units, indicating the vertical dimension should be included in at least a 2-layer model,
Dye cloud spreads in non-Gaussian manner	- some differential shearing is present and system should be studied using a multi-layer model, or reserve judgment to the calculations in Step 6, and
Dye cloud moves downstream and diffuses in a Gaussian manner	- little differential shearing is present and system could be modeled neglecting vertical dimension after calculations in Step 6.



a) Tidal Velocity Reversal



b) Residual Velocity Reversal



c) No Observable Reversals

Figure IV-6 VERTICAL VELOCITY PROFILES

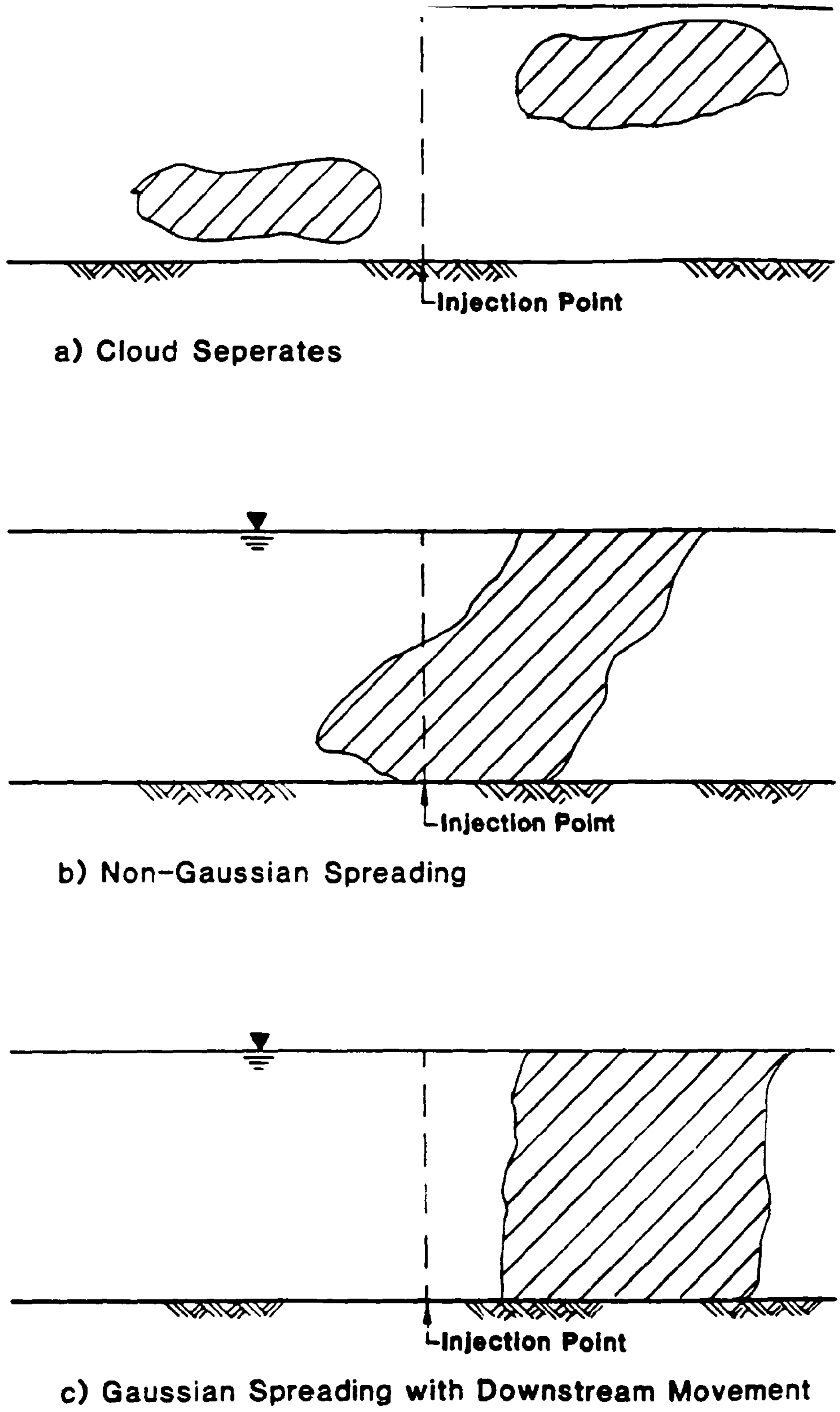


Figure IV-7 VERTICAL DYE CONCENTRATION PROFILES

Geomorphological Classification

If little or no data is present, one can try to categorize the estuary within the basic definitions of Dyer (1973). Over the years, a systematic structure of geomorphological classification has evolved. Dyer (1973) and Fischer et al. (1979) identify four groups:

- o Drowned river valleys (coastal plain estuaries),
- o Fjords
- o Bar-built estuaries, and
- o Other estuaries that do not fit the first three classifications.

Typical examples of North American estuaries are presented in Tables IV-1 and IV-2.

Coastal plain estuaries are generally shallow with gently sloping bottoms, and depths increasing uniformly towards the mouth. Such estuaries have usually been cut by erosion and are drowned river valleys, often displaying a dendritic pattern fed by several streams. A well-known example is Chesapeake Bay. Coastal plain estuaries are usually moderately stratified (particularly in the old river valley section) and can be highly influenced by wind over short time scales.

Bar built estuaries are bodies of water enclosed by the deposition of a sand bar off the coast through which a channel provides exchange with the open sea, usually servicing rivers with relatively small discharges. These are often unstable estuaries, subject to gradual seasonal and catastrophic variations in configuration. Many estuaries in the Gulf Coast and Lower Atlantic Regions fall into this category. They are generally a few meters deep, vertically well mixed and highly influenced by wind.

Fjords are characterized by relatively deep water and steep sides, and are generally long and narrow. They are usually formed by glaciation, and are more typical in Scandinavia and Alaska than the contiguous United States. There are examples along the Northwest Pacific Coast, such as Alberni Inlet

TABLE IV-1. TOPOGRAPHIC ESTUARINE CLASSIFICATION

Type	Dominant Long-Term Process	Vertical Degree of Stratification	Lateral Variability	Examples
Coastal Plain	River Flow	Moderate	Moderate	Chesapeake Bay, MD/VA James River, VA Potomac River, MD/VA Delaware Estuary, DE/N New York Bight, NY
Bar Built	Wind	Vertically well mixed	High	Little Sarasota Bay, F Apalachicola Bay, FL Galveston Bay, TX Roanoke River, VA Albemarle Sound, NC Pamlico Sound, NC Puget Sound, WA
Fjords	Tide	High	Small	Alberni Inlet, B.C. Silver Bay, AL
Other Estuaries	Various	Various	Various	San Francisco Bay, CA Columbia River, WA/OR

TABLE IV-2. STRATIFICATION CLASSIFICATION

Vertical Type	Lateral Type	River Discharge	Examples
Highly Stratified	Laterally homogeneous	Large	Mississippi River, LA Mobile River, AL
Partially Mixed	Partially mixed	Medium	Chesapeake Bay, MD/VA James Estuary, VA Potomac River, MD/VA
Vertically Homogeneous	High Variability	Small	Delaware Bay, DE/NJ Raritan River, NJ Biscayne Bay, FL Tampa Bay,FL San Francisco Bay, CA San Diego Bay, CA

in British Columbia. The freshwater streams that feed a fjord generally pass through rocky terrain. Little sediment is carried to the estuary by the streams, and thus the bottom is likely to be a clean rocky surface. The deep water of a fjord is distinctly cooler and more saline than the surface layer, and the fjord tends to be highly stratified.

The remaining estuaries not covered by the above classification are usually produced by tectonic activity, faulting, landslides, or volcanic eruptions. An example is San Francisco Bay which was formed by movement of the San Andreas Fault System (Dyer, 1973).

Using this classification, the approach is to estimate the degree of stratification from known conditions in a geomorphologically similar estuarine and use the criteria under a "degree of stratification" given above.

IV.3.2 LATERAL DIMENSION

Neglecting the lateral dimension in the far field is more difficult to estimate than for the vertical dimension, although the same features can be considered. These are:

- o salinity and/or temperature gradients,
- o tidal or residual velocity reversals,
- o dye cloud splitting and differential advection, and/or
- o geomorphological classification.

The analyses in this step are the same as for the vertical dimension analyses (no equivalent to the stratification diagram exists) except that we are looking for lateral gradients and reversals. Using the geomorphological classification, the reader should refer to Tables IV-1 and IV-2.

IV.4 PROCESS TIME AND SPACE SCALES

At this point we begin to narrow our attention to time and spatial scales compatible with physical/chemical/biological processes and at which resolution of predicted results is desired. It is important at this step to refer to the conceptual model, developed in Step 1, of the important processes which should be included in the numerical model. This is necessary for two reasons. Firstly, it provides a checklist of processes or variables included in the final numerical model selected. If the checklist is not completely satisfied, the shortfall can be used to assess the need for further model modification/development, or a comprise achieved and a revised conceptual model developed. Secondly, it can be used as a base to estimate rate coefficients used in defining process linkages in the numerical model. As we have said, an important consideration in selecting an appropriate numerical model is the question of dynamic versus steady-state modeling. It is intuitively evident that some measure of the ratio of physical-to-biochemical rates (perhaps defined by flushing time divided by a measure of kinetic rates, such as the smallest T_{90}) can be used to make this assessment.

In order to more closely investigate the possibility of reducing model dimensionality, we must be able to understand the time and space scales of the physical/chemical/biological processes included in the conceptual model of the prototype system, and their interrelationships. To do this, we will define only physical and chemical time and space scales as:

- physical - flushing time
- biochemical - biochemical reaction, decay, and dieoff rate.

IV.4.1 FLUSHING TIME

The time that is required to remove pollutant mass from a particular point in an estuary (usually some upstream location) is called the flushing time. Long flushing times are often indicative of poor water quality conditions due to long residence times for pollutants. Flushing time, particularly in a segmented estuary, can also be used in an initial screening of alternate locations for facilities which discharge constituents detrimental to estuarine health if they persist in the water column for lengthy periods.

Factors influencing flushing times are tidal ranges, freshwater inflows, and wind. All of these forcing functions vary over time, and may be somewhat unpredictable (e.g., wind). Thus, flushing time calculations are usually based on average conditions of tidal range and freshwater inflows, with wind effects neglected.

The Fraction of Fresh Water Method for flushing time calculation is based upon observations of estuarine salinities:

$$F = \frac{S_o - S_e}{S_e} \qquad \text{(IV-8)}$$

where F = flushing time in tidal cycles,
S_o = salinity of ocean water, and
S_e = mean estuarine salinity.

The tidal prism method for flushing time calculation considers the system as one unit with tidal exchange being the dominant process:

$$F = \frac{V_L + P}{P} \qquad \text{(IV-9)}$$

where F = flushing time in tidal cycles,
V_L = low tide volume of the estuary, and
P = tidal prism volume (volume between low and high tides).

The Tidal Prism technique was further modified by Ketchum (1951) to segment the estuary into lengths defined by the maximum excursion of a particle of water during a tidal cycle. This technique can now include a freshwater inflow:

$$F = \sum_{i=1}^{n} \frac{V_{Li} + P_i}{P_i} \qquad \text{(IV-10)}$$

where
F = flushing time in tidal cycles,
i = segment number,
n = number of segments
V_{Li} = low tide volume in segment i, and
P_i = tidal prism volume in segment.

Riverine inflow, Q_R, is accounted for by setting the upstream length equal to the river velocity multiplied by the tidal period, and setting:

$$P_o = Q_R T \qquad \text{(IV-11)}$$

where
P_o = tidal prism volume in upstream segment,
Q_R = freshwater flow, and
T = tidal period.

Finally, the replacement time technique is based upon estuarine geometry and longitudinal dispersion:

$$t_R = 0.4\ L^2/E_L \qquad \text{(IV-12)}$$

where
t_R = replacement time,
L = length of estuary, and
E_L = longitudinal dispersion coefficient.

This technique requires knowledge of a longitudinal dispersion coefficient, E_L, which may not be known from direct estuarine measurements. A coefficient based upon measured data from a similar estuary may be assumed (see Table IV-3 for typical values in a number of U.S. estuaries) or it may be estimated from empirical relationships, such as the one reported by Harleman (1964):

$$E_L = 77\ n\ u\ R^{5/6} \qquad \text{(IV-13)}$$

TABLE IV-3

OBSERVED LONGITUDINAL DISPERSION COEFFICIENTS

Estuary	River Flow	Dispersion Coefficents	
	(cfs)	(m^2/sec)	(ft^2/sec)
Delaware River (DE/NJ)	2500	150	1600
Hudson River (NY)	5000	600	6500
East River (NY)	0	300	3250
Cooper River (SC)	10000	900	9700
Savannah River (GA, SC)	7000	300-600	3250-6500
Lower Raritan River (NJ)	150	150	1600
South River (NJ)	23	150	1600
Houston Ship Channel (TX)	900	800	8700
Cape Fear River (NC)	1000	60-300	650-3250
Potomac River (MD/VA)	550	30-300	325-3250
Compton Creek (NJ)	10	30	325
Wappinger and Fishkill Creek (NY)	2	15-30	160-325
San Francisco Bay (CA):			
Southern Arm	-	18-180	200-2000
Northern Arm	-	46-1800	500-20000

SOURCE: From Mills et al. (1982).

or Harleman (1971):

$$E_L = 100\ n\ u_{max}\ R^{5/6} \qquad \text{(IV-14)}$$

where E_L = longitudinal dispersion coefficient (ft^2/sec),
n = Manning's roughness coefficient (0.028-0.035, typically),
u = velocity (ft/sec),
u_{max} = maximum tidal velocity (ft/sec), and
R = hydraulic radius = A/P (ft)

where A = cross sectional area (ft),
P = wetted perimeter (ft).

V.4.2 DECAY OF DIEOFF RATES

A measure of biochemical process time scales is given by the decay rate, K, or the dieoff rate, usually denoted by T_{90}. T_{90} is defined as the time to reduce the constitutent concentration by an order of magnitude, or 90 percent. The relationship between the two is:

$$T_{90} = 2.3/K \qquad \text{(IV-15)}$$

where T_{90} = dieoff rate in hours, and
K = decay rate in 1/hours.

Of critical concern in selecting a water quality model is the ability to resolve the most rapid constituent dieoff. Thus, from a knowledge of the system chemistry, select the minimum dieoff rate T_{90}^{min} as the biochemical process time scale. If there is a large difference between two rates (e.g., 10 mins versus 24 hours), we may want to consider neglecting one or the other of the processes in the conceptual model (Section IV.1).

IV.5 REGULATORY SCALES

It is important to make a clear statement of the purpose and objectives of a study. Frequently, such a statement is bound to local/state/federal regulations which, in turn may imply time and spatial scales that must be resolved by the model description. An example of this is the concept of an "allowable mixing zone" frequently defined in the vicinity of an outfall. The regulation may be so written that the numerical model must have sufficient spatial resolution to determine that the mixing zone length is not exceeded (thus requiring distance steps at least an order-of-magnitude less than this length) and that no violations occur at any time, which may necessitate a dynamic rather than steady state approach to modeling.

More often than not, the purpose of modeling is to evaluate compliance with Federal or State regulations. Many of these regulations define time and space scales beyond which violations will not be permitted. For example, the regulation for a thermal outfall may state that waters must return to within 2°C of the ambient temperature after 100 m downstream in the river. This clearly defines a length scale of 100 m, and a time scale of 100 m divided by the ambient river velocity.

Thus, if regulatory standards are a consideration in the model selection process, we will define a regulatory length scale, L_R as:

L_R = the minimum of the specified distance if known from regulations, length of system wished to be modeled, or total length of system, (IV-16)

and a time scale, T_R as:

$$T_R = L_R/\bar{\bar{u}} \qquad \text{(IV-17)}$$

where $\bar{\bar{u}}$ = velocity averaged over time and space scales.

IV.6 STUDY SCALE DIMENSION REDUCTION

Based on the information of Steps 1-5, we can now develop a more refined conceptual model that incorporates all the information of these steps. The emphasis in this step is to determine whether spatial dimensions, other than those determined non-negligible in Step 3, can be neglected and yet resolve all necessary physical/chemical/biological processes at the regulatory spatial scale.

As an example of this, consider wastewater discharged into a stratified estuary. Step 3 may show that stratification is important and thus the vertical variation cannot be neglected (or integrated). However, the question may still remain whether it is reasonable to neglect lateral variations and assume a laterally well-mixed system. If the regulations reviewed in Step 5 require a mixing zone of not more than 1000 m downstream of the outfall, we would wish to determine from this step whether the laterally well-mixed condition is reached before or after this distance. If it is reached before 1000 m, for example, it may be reasonable to neglect lateral variations, However, if it is reached afterwards, the lateral dimension is still required to be able to adequately compare simulated results with the regulatory standard.

In Step 3 (Section IV.3), we looked at the irreducability of dimensions at the far field scale. This included analyses and subjective indications that considered:

- Density stratification,
- Velocity data,
- Dye studies, and
- Topographic characteristics.

These were included at the far field level because such data are usually either unavailable in the potential study area or are inadequate to make a reliable determination of dimension reductions at this scale. Normally any data in the study area will be part of a larger data set covering a much wider area.

Having identified the dimensions we should not neglect, from Step 3, in this step we wish to determine whether any of the other dimensions can be neglected. Having probably exhausted our supply of data to make such determinations, we will rely on simple analytic solutions.

At this stage, we should have a fairly complete conceptual model of the system to be studied. This should include a definition of the minimum study spatial resolution, L_S, defined as the minimum of the process space scale, L_p, and the regulatory space scale, L_R:

$$L_S = \min (L_p, L_R) \tag{IV-18}$$

There are three dimension reductions we will consider here:

1. Cross-sectional area,
2. Vertical dimension, and
3. Lateral dimension.

There are several techniques that can be used to make these assessments:

- o Fischer's mixing length, and
- o Analytic transport models.

Fischer's Mixing Length

A frequently used technique described by Fischer et al. (1979) is to use a definition of the convective length, L_c, over which the discharge plume is completely mixed laterally, so that "the concentration is within 5 percent of its mean value everywhere in the cross section" for a centerline discharge:

$$L_c = 0.1\ u\ W^2/E_y \tag{IV-19}$$

where u = mean velocity, (L/T)
W = channel width, (L), and
E_y = lateral diffusion coefficient.

For a side discharge, W is replaced with 2W for symmetry:

$$L_c = 0.4\ u\ W^2/E_y \tag{IV-20}$$

A good estimate (Fisher et al., 1979) for the lateral diffusion coefficient, Ey, is:

$$E_y = 0.6\ R\ u^* = 0.06\ R\ u \qquad \text{(IV-21)}$$

where R = hydraulic radius, (L), and
u^* = bed shear velocity, (L/T)

Thus, for a centerline discharge:

$$L_c = 6.67W^2/R \qquad \text{(IV-22)}$$

and for a side discharge:

$$L_c = 26.67W^2/R \qquad \text{(IV-23)}$$

If the convective length, L_c, is less than the study space scale, L_S, a cross sectionally averaged model can be selected.

Analytical Model

A second technique, which is actually more general in the sense that it can be directly related to the definition of complete mixing (Step 2), is to use a closed form (analytic) solution to the governing three-dimensional mass transport equation (Eq. II-5). To obtain a closed form solution, the following assumptions are made:

1. the velocity, u, is steady and uniform over the entire cross section (or layer if analyzed specifically as such),
2. the load is either (a) an instantaneous point source, or (b) a continuous point source,
3. the diffusion coefficients, Ex, Ey, Ez are constant in space and time, and
4. reflections of the solution at solid and surface boundaries can be accounted for using a series of image sources (Figure IV-8),

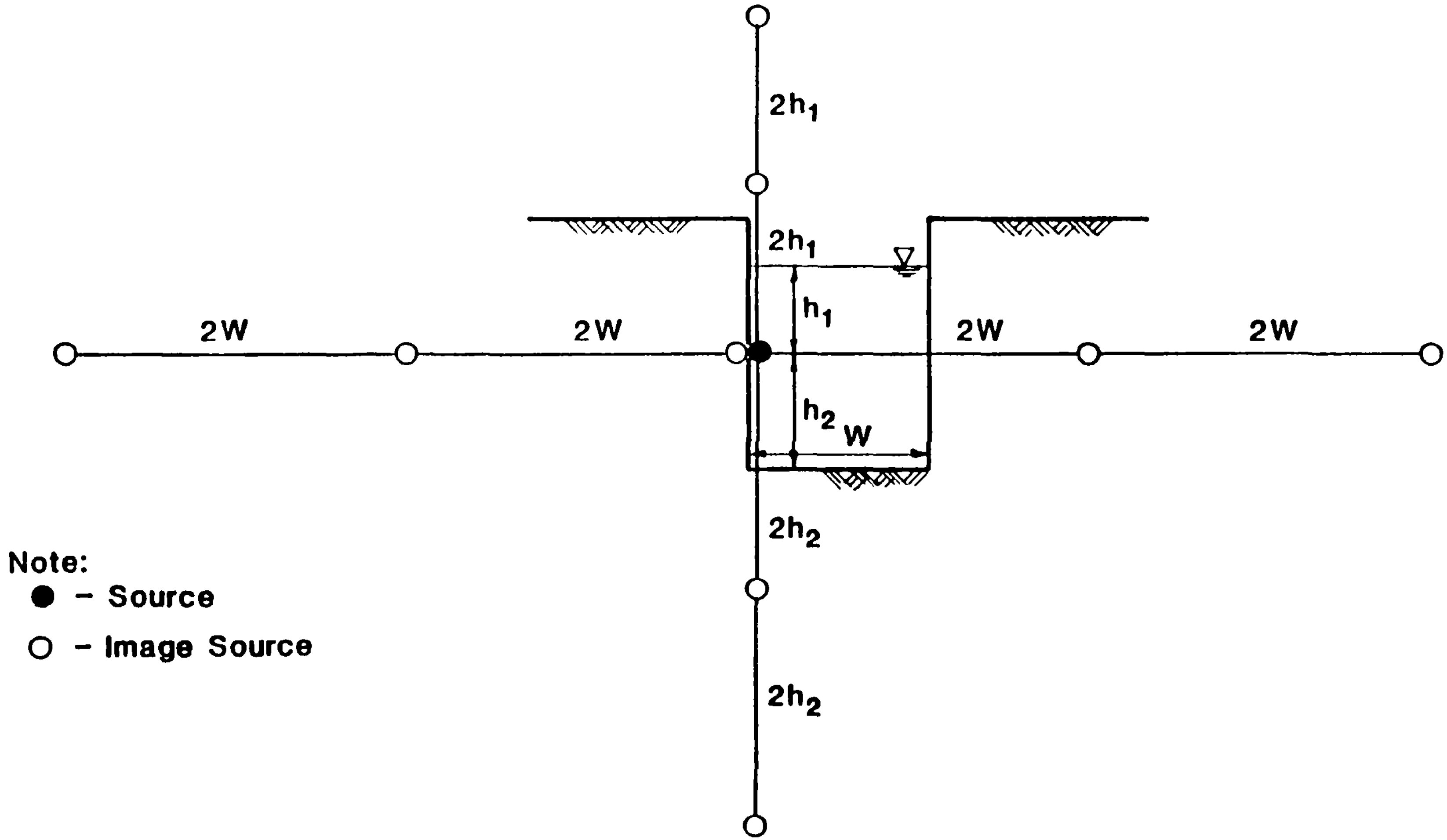


Figure IV-8 SCHEMATIC OF SOURCE AND IMAGE SOURCES

Then (using Fisher et al., 1979) the instantaneous point source distribution is:

$$c(x,y,z,t) = \sum_{j=-J}^{J} \sum_{k=-K}^{K} \left\{ \frac{M}{(4\pi t)^{3/2} \; (E_x E_y E_z)^{1/2}} \exp - \left[\frac{(x-x_i-ut)^2}{4E_x t} + \frac{(y-y_i)^2}{4E_y t} + \frac{(z-z_i)^2}{4E_z t} - K_D t \right] \right\} \qquad \text{(IV-24)}$$

where $c(x,y,z,t)$ = concentration at location x,y,z (within the channel) at time t,

M = mass load (M),

ρ = mass density, (M/L^3)

E_x, E_y, E_z = longitudinal, lateral, and vertical diffusion coefficients, (L^2/T)

j = -J, J is number of lateral image sources (Figure IV-8)

k = -K, K is number of vertical image sources (Figure IV-8)

x_i, y_i, z_i = location of each image (or actual source), and

K_D = decay coefficient, (1/T).

Similarly, the steady-state concentration distribution, $c(x,y,z)$, for a continuous point source is:

$$c(x,y,z) = \sum_{j=-J}^{J} \sum_{k=-K}^{K} \left\{ \frac{q}{4\pi\rho \; (E_y E_z)^{1/2} \; ((x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2)^{1/2}} \exp - \left[\frac{((x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2)^{1/2} \; (u^2 + 4(E_y E_z)^{1/2} K_D)^{1/2} - u(x-x_i)}{2(E_y E_z)^{1/2}} \right] \right\} \qquad \text{(IV-25)}$$

where q = mass loading rate, (M/T)

If the diffusion coefficients are unknown, they can be estimated from (Fischer et al., 1979):

$$E_x = 0.6 \; R \; u^* \quad \text{(assumed equal to the lateral coefficient)}$$

$$E_y = 0.6 \; R \; u^* = 0.06 \; R \; u \qquad \text{(IV-26)}$$

$$E_z = 0.067\ R\ u^* = 0.0067\ R\ u$$

where u^* = bed shear velocity

The procedure is to:

1. Select either an instantaneous point source or a continuous point source,

2. estimate velocity, loads, and diffusion coefficients,

3. select a number of image sources (usually J = K = 3 will be adequate),

4. use the appropriate equation above (IV-24 or IV-25) and calculate cross-sectional distribution,

5. find the closest sections (both vertically and laterally) that satisfy the definition of complete mixing from Step 2, and

6. compare those distances, L, to the sections with the minimum spatial resolution needed (Eq. IV-18). If $L < L_S$ the dimension considered can be assumed to be well mixed and neglected for model selection purposes. If $L < L_S$, the section will not be completely well-mixed, and the dimension must be included in the selected model description.

IV.7 DYNAMIC OR STEADY-STATE

Again based on the information of Steps 1-6, we further wish to make a decision whether a steady-state model can be used or whether a dynamic model is required to achieve the required temporal resolution. An example of this is that the dissolved oxygen (DO) standard in many states requires no oxygen depletion below a given level at any time. In a tidal river, for example, in which processes can occur within or at the same period as a tidal cycle (many constituents will exhibit diurnal variations which are not in phase with the tidal cycle) a dynamic model may be required to provide adequate temporal resolution to make such a determination.

Steady-state modeling is inherently more economical than dynamic modeling. Another advantage is that it can perhaps be adapted to run on a microcomputer for relatively simple kinetic descriptions, thus making the approach more readily available to groups with severe computer hardwater limitations. Finally, steady-state models are usually less complex, because the cumbersome hydrodynamic equations have been greatly simplified to include only the continuity equation.

There is a great danger, however, of choosing such an approach without considering the implications of the selection. It is intuitively argued that a steady-state approach is of little use in a closed-end canal system, for example, because there is no (or at least, very little) net advection towards the mouth. By contrast, one would frequently choose such an approach for a stream with no tidal effect. But what about the systems in between -- those that have both net downstream advection and tidal oscillations?

Unfortunately, there is no hard and fast rule that can be applied. Rather we must rely on our experience, plus some obvious physical/chemical process limits. It seems reasonable that a decision criteria would depend on the time scales of both physical and biochemical rates, most likely as a ratio. Physical time scales, T_p, will be defined as the minimum of the tidal period, T, and the flushing time, F:

$$T_p = \min (T,F) \tag{IV-27}$$

The biochemical process time scale, T_c, is defined as the minimum of the kinetic rates, using the concept of an order-of-magnitude or 90% reduction, T_{90}, and any regulatory time scale, T_R, defined in Step 5:

$$T_c = \min (T_{90}, T_R) \tag{IV-28}$$

Defining the ratio:

$$R = T_p/T_c \tag{IV-29}$$

we would recommend the following criteria:

- o If $R > 0.5$ - use a dynamic model
- o If $R < 0.1$ - use a steady-state model
- o If $0.1 < R < 0.5$ - selection should be based on other factors such as sensitivity of the study, reliability of available data, cost, etc.

IV.8 SPATIAL AND TEMPORAL RESOLUTION

The selection of space and time steps for the numerical model is intended to provide sufficient resolution to adequately describe the physical/chemical/biological processes included in the model description. However, in many cases, this selection must also include a consideration of model accuracy and stability.

IV.8.1 RESOLUTION

To ensure adequate temporal resolution of processes included within the model description, the time step, Δt, must be less than the time scale of the model, T_S, defined as the length scale, L_S, divided by a characteristic system velocity. Such a selection can be semi-intuitive. For example, consider the number of piece-wise continuous straight lines that can approximate a sine curve over a tidal cycle. In general, we would recommend:

$$\Delta t < 0.1\ T_S \tag{IV-30}$$

In a similar manner, the space step, characterized perhaps by its longitudinal value, Δx, must be adequate to resolve spatial distributions. In general, Δx should be smaller for larger concentration gradients, and can be larger away from such areas (if the numerical scheme can offer that type of flexibility). Higher concentration gradients are likely to be found near waste sources, and decrease away from them. To estimate spatial resolution then, one can use the calculations of step 6 (Section IV.6), and approximate the resulting distribution with a series of piece-wise lines until an adequate representation results. The minimum spatial resolution required, Δx_{min}, can be determined from the resulting construction (Figure IV-9).

IV.8.2 STABILITY

Most computer waste load allocation models use explicit schemes--that is, variables at the new time level are calculated using known values at previous time levels. This leads to several common conditions that must be satisfied to ensure model stability (i.e., solutions remain within bounds and do not "blow up"). Furthermore, satisfying these conditions will often result in smaller time steps that would generally be needed from solution resolution conditions alone.

These conditions, or criteria for a one-dimensional are usually, a hydrodynamic criterion (Courant condition):

$$\Delta t \leq \frac{\Delta x}{\sqrt{gh} \pm u} \qquad \text{(VI-31)}$$

a mass transport condition:

$$\Delta t \leq \frac{\Delta x}{u} \qquad \text{(VI-32)}$$

and a dispersion condition:

$$\Delta t \leq \frac{\Delta x^2}{4E_L} \qquad \text{(VI-33)}$$

Similar conditions exist for 2 and 3-dimensional models, and other conditions, such as a friction term criterion, may also be required. The most stringent condition is usually the Courant condition (unless vertical diffusion and/or momentum transfer is explicitly treated, in which case a criterion like Equation (IV-32) is required with Δz replacing Δx). Some

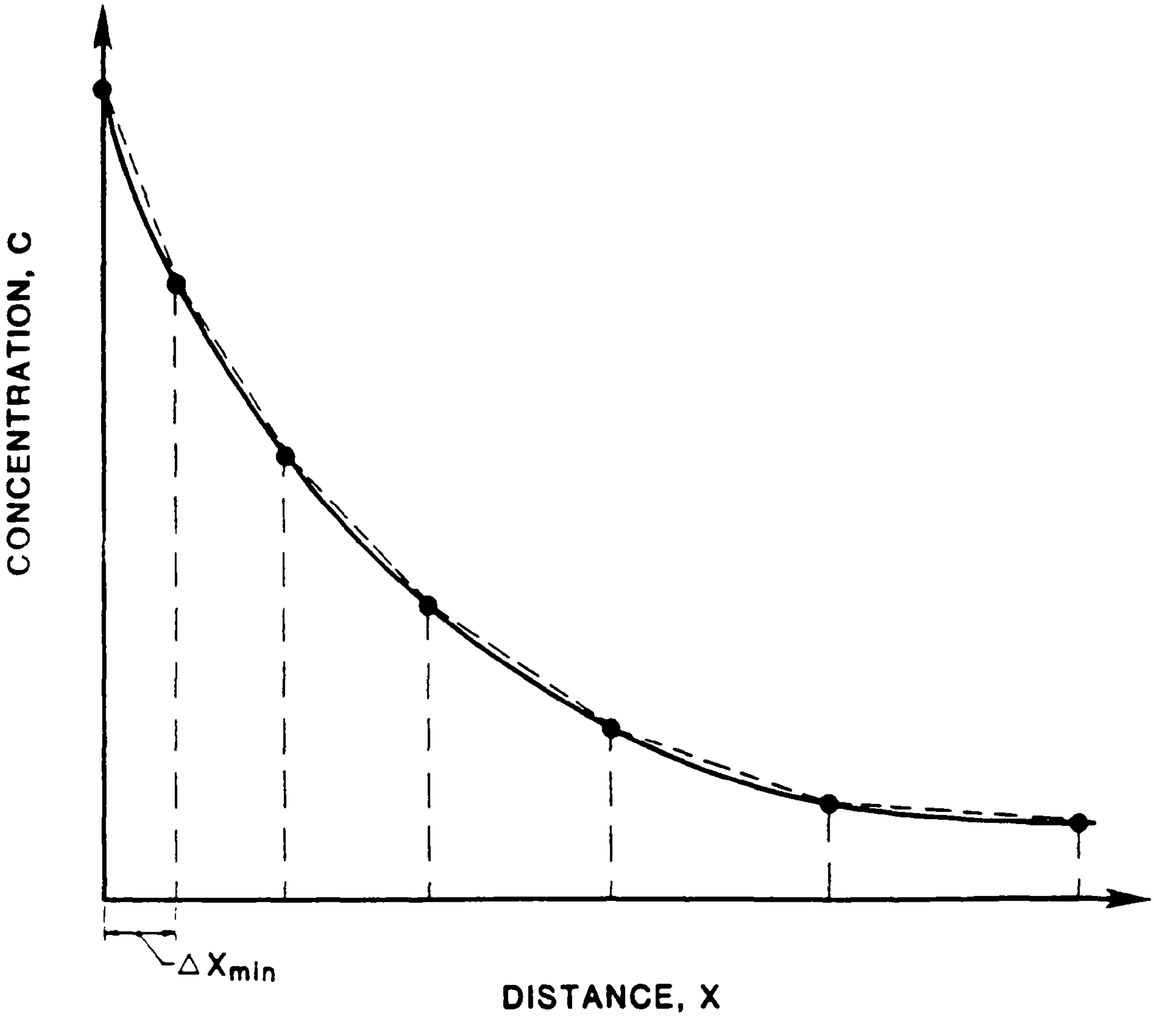


Figure IV-9. APPROXIMATION TO CONCENTRATION GRADIENT models may solve for the mass transport in a separate model, or at a different time step than the hydrodynamic solution. In these cases, all the above criteria should be checked.

Some models exist which use an implicit technique to approximate the governing equations. In these cases, the model may be unconditionally stable, which means that the choice of the time step is not limited by stability considerations. Here, the time step should be chosen to provide adequate resolution of temporal processes.

IV.9 DIFFUSION COEFFICIENTS

In dynamic modeling, the choice of the form to describe the diffusion process is fairly standard, as discussed in Section II.9. As further discussed in that Section, the selection of diffusion coefficients for steady-state models is much less well-defined, and frequently in error, or at least not well based. In this Step, we will recommend an approach to diffusion coefficient selection for steady-state models, based on some physical aspects of the system being studied.

Diffusion coefficient selection for dynamic models is both straightforward, in that the form used in any particular model selected will probably be adequate, and yet, at the same time, to establish rigorous guidelines as to the most appropriate form is very difficult. Our advice here is to follow the discussion of Section II.9 and ensure that the form used in a particular model has a reasonably sound basis. In most cases, as a dynamic model is complex, and usually well reviewed (choosing well-known models or agency-supported models can lead to increased confidence), one may generally assume that it contains an adequate description of the diffusion processes. Furthermore, diffusion in a dynamic model is not as critical as dispersion in a steady-state model, in which neglected processes are inherently lumped into the dispersion mechanism.

More care must be exercised when selecting the appropriate dispersion coefficient description to be used in a steady-state model. Such a selection, as has frequently been stated in this report, must be based on a sound knowledge of the physical/chemical processes at work and the inherent assumptions made when the hydrodynamic equations are simplified or time integrated.

Following the discussion of Section II.9, there are three types of tidally-averaged dispersion coefficients, E_L^T, commonly used in steady-state models:

1. E_L^T = constant (space, time) (IV-34)

2. E_L^T = constant (time) (IV-35)

3. $E_L^T = KRQ_R/A$ (IV-36)

Selection of the most appropriate form will be based on a consideration of the respective influences of river and tidal flows. In general, we would recommend that Eq. (IV-35) be used for tidally dominated flows, Eq. (IV-35) bee used for river dominated flows, and Eq. (IV-35) be used as little as possible or when no data is available for a more rational selection.

More specifically, we propose the following criteria:

- o If river flow is strong enough that the estuarine flow is always unidirectional i.e. (from Eq. II-24):

$$Q_R > A_{ws} aw \qquad \text{(IV-37)}$$

where Q_R = river flow, (L^3/T),

A_{ws} = upstream water surface area, (L^2),

a = tidal amplitude, (L), and

w = $2\pi/T$, $(1/T)$,

where T = tidal period,

then use:

$$E_L^T = KRQ_R/A \qquad \text{(IV-38)}$$

where A = cross-sectional area.

- If the tidal flows dominate, such that the river flow is less than 10% of the maximum tidal flow:

$$Q_R < 0.1 A_{ws} aw \qquad \text{(IV-39)}$$

then use:

$$E_L^T = \frac{4aA_{ws}KR}{TA} \qquad \text{(IV-40)}$$

- If the flow is some intermediate combination of river and tidal flows:

$$0.1 < Q_R/A_{ws}aw < 1.0 \qquad \text{(IV-41)}$$

then Eqs. (II-25) and (II-26) can be used as a guide for coefficient form selection, for:

$$t_1 \text{ and } t_2 = \frac{1}{w} \sin^{-1}\left[\frac{Q_R}{awA_{ws}}\right] \quad \text{for } 0 \leq t \leq T \qquad \text{(IV-42)}$$

$$E_L^T = \frac{KR}{TA}\left[Q_R\,(T + 2t_1 - 2t_2) + 2aA_{ws}\,(1 + \cos(wt_1) - \cos(wt2))\right] \qquad \text{(IV-43)}$$

It should be noted that the above analyses may not apply everywhere is a given system. Consider the Potomac River, for example. Upstream, the river is strongly tidal and Eq. (IV-38) can be applied. Downstream, the river may dominate and Eq. (IV-40) can be applied. In the middle reaches, there is a balance between river and tidal flows, and thus Eq. (IV-43) can be used as a guide.

IV.10 DATA AVAILABILITY

At this point, the model selection procedure should have arrived at the point where the processes, dimensionality, and time scales are determined.

The next step is then to consider whether sufficient data exist to run the model.

These data are required for two purposes--calibration and verification. Calibration is a process of adjusting model coefficients, until good agreement is achieved between simulation and observations. The measures of "goodness-of-fit" may be either judgmental or statistical, using such approaches as relative errors, root-mean-square errors, and tests of statistical significance of variations, etc. Model verification then requires that a second data set be simulated, without adjusting model coefficients, to demonstrate that the model can accurately reproduce a (preferably) different set of conditions.

If sufficient data do not exist, a decision must be made to (a) collect additional data to supplement existing data, or (b) to use the existing data to perform model calibration only. This latter condition is not desirable because it must reduce confidence in the model's ability to accurately simulate conditions other than those found during calibration. Perhaps the most desirable situation is to have three of four data sets covering a wide range of conditions to be used for calibration and verification.

IV.11 MODEL SELECTION

Having completed Steps 1-10 (Section IV.1-IV.10), the system to be studied should be comprehensively conceptualized. At this point, we are able to select the most appropriate model to do the job. As a basis for model selection, a "check list" should be prepared of desired model features, with room to evaluate the features of several candidate models. A sample list is shown in Table IV-4 as a guide.

The ability to perform this model selection does not only depend on one's capability of evaluating Steps 1-10, but also on the knowledge of available numerical models that are possible candidates. Most "experienced" modelers will process this knowledge, and one commonly held view is that only experieced modelers should use models. Certainly there is a great danger in an inexperienced modeler or team of modelers performing a study.

TABLE IV-4

EXAMPLE MODEL SELECTION CHECKLIST

Category	Item	Conceptual Model	Model 1	Model 2	Model 3
Dimensions	Longitudinal (x) lateral (y) vertical (z)				
Time Integration	Dynamic steady-state				
Dispersion Cofficient	Constant (x, t) tidal dominated river dominated				
Physical features	Coriolis nonlinear acceleration bottom friction wind shear variable water surface density				
Chemical constituent	Constituent a Constituent b				
Chemical kinetics	Kinetic 1 Kinetic 2				
Solution scheme	Finite difference Finite element link node				

However, the current trend is to consider the model as a "black box" and to use it with as much guidance as can be provided in reports such as this, authored by experienced modelers.

To those inexperienced in model use or those who are unfamiliar with models in a certain area of estuarine hydraulics/water quality modeling, there is no one central agency to which one can turn to provide a complete summary of available models. Such a mechanism does exist in groundwater modeling through the Holcomb Research Institute at Butler University in Indianapolis. Termed "a clearing house", one of its functions is to provide a library service of available software for groundwater modeling. Such a mechanism is being considered for hydraulics/hydrology by the American Society of Civil Engineers Task Committee on the Documentation of Hydraulic Software, but the implementation of any such recommendation is still some time away.

There are several ways one might approach the task of actual model selection:

1. Use models that are readily available to the user or lie within their realm of experience,

2. Perform a library search, perhaps using a computerized database, such as DIALOG,

3. Seek the advise of a knowledgeable modeler, and

4. Reference bibliographic and/or model specific reports and papers.

Most model users usually have both a basis of experience and access to knowledgeable modelers. Once Steps 1-10 have been performed, and several candidate models identified, final model selected is based on previous experience with various models. Factors such as ease of use, reliability, accuracy, availability, and economy can be weighed in choosing the model.

Without such a basis of knowledge, or when a particular study is beyond one's previous experience, model selection follows ways 2-4, above. In particular, there are a number of bibliographic and model selection summary reports that one might turn to for information (e.g., EPA, 1979; Versar, 1983; JRB, 1984; Ambrose et al., 1981; etc.).

A good example of a comprehensive discussion of estuarine waste load allocation models is the study by Ambrose et al. (1981). They divided estuarine waste load allocation models into four levels according to the following definitions:

Level I includes desktop screening methodologies which calculate seasonal or annual mean pollutant concentrations based on steady state conditions, simplified flushing time estimates, and first order decay coefficients. These models are designed to examine an estuary rapidly to isolate trouble spots for more detailed analyses. They should be used to highlight major water quality issues and important data gaps.

Level II includes computerized steady state or tidally averaged planning models which generally use a box or compartment-type network. Steady state models use an unvarying flow condition which neglects the temporal variability of tidal heights and currents. Tidally averaged models simulate the net flow over a tidal cycle. These models cannot predict the variability and range of DO and pollutants throughout each tidal cycle, but they are capable of simulating variations in tidally averaged concentrations over time. Level II models can predict slowly changing seasonal water quality with an effective time resolution of two weeks to a month.

Level III includes computerized one-dimensinal (1-D) and quasi two-dimensional (2-D), real time planning models. These real time models simulate variations in tidal heights and velocities throughout each tidal cycle. One-dimensional models treat the estuary as well-mixed vertically and laterally.

Quasi 2-D models employ a link-node approach which describes water quality in two dimensions (longitudinal and lateral) through a network of 1-D nodes and channels. The 1-D equation of motion is applied to the channels while the continuity equation is applied at nodes between channels, where all the storage is assumed to be concentrated. Tidal movement is simulated with a separate hydrodynamic package in these models. Although the Level III models will calculate hour-to-hour changes in water quality variables, their effective time resolution is usually limited to one week because tidal input parameters generally consist of only average or slowly varying values. Model results should be averaged to obtain mean diurnal variability over a minimum of one week intervals within the simulated time period (Ambrose and Roesch, 1982).

Level IV consists of computerized 2-D and 3-D real time design models. Dispersive mixing and seaward boundary exchanges are treated more realistically than in the Level III 1-D models. At the present time, there are no well-documented three-dimensional water quality models which include coupled constituent interactions and feedback reactions. The only 3-D models currently reported in the literature are hydrodynamic models that include simple first order decay rates for uncoupled nonconservatives (Swanson and Spaulding, 1983). The only well-documented 2-D estaurine water quality models simulate quality and hydrodynamics in the lateral and longitudinal directions, but it is also possible to develop a fully two-dimensional model in the longitudinal and vertical directions. The effective time resolution of the Level IV models is less than one day with a good representation of diurnal water quality and intratidal variations.

JRB (1983) provides a discussion of the advantages and disadvantages of Level I-IV models. However, the aim of the model selection process described in this section, is to choose the model with the minimum set of features that adequately describes the prototype situation. This automatically leads to the selection of the most appropriate and most economic model, based on the assumption (usually true) that more complex models are more costly.

The procedure discussed in Steps 1-10 above, can be tied into the Levels of Ambrose et al. (1981), quite simply through the required dimensionality and time integration required in the study. The classification of Level I-IV models is purely based on model dimensions and whether the model is steady-state or dynamic.

In summary, the model selection procedure is:

1. Perform the analyses of Steps 1-10 (Sections IV.1-IV.10) and compile a model feature "checklist", such as Table IV-4,

2. Identify a number or source of relevent models,

3. List these models features on the "checklist" (Table IV-4),

4. List those models which provide the required features and make a final decision based on such factors as availability, previous experience, training, documentation, cost, compatibility with computers, etc, and

5. If no such model exists, decide to (a) modify the most appropriate model to include the missing features, or (b) redefine the objectives, and thus the conceptual model, or the study to fit the most appropriate model found.

SECTION V

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