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RATES, CONSTANTS, AND KINETICS FORMULATIONS IN SURFACE WATER QUALITY MODELING (SECOND EDITION)

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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient analytical tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Technology Development and Applications Branch develops management or engineering tools to help pollution control officials achieve water quality goals.

Basin planning requires a set of analysis procedures that can provide an assessment on the current state of the environment and a means of predicting the effectiveness of alternative pollution control strategies. This report contains a revised and updated compilation and discussion of rates, constants, and kinetics formulations that have been used to accomplish these tasks. It is directed toward all water quality planners who must interpret technical information from many sources and recommend the most prudent course of action that will minimize the cost of implementation of a pollutant control activity and maximize the environmental benefits to the community.

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ABSTRACT

Recent studies are reviewed to provide a comprehensive volume on state-of-the-art formulations used in surface water quality modeling along with accepted values for rate constants and coefficients. Topics covered include: dispersion, heat budgets, dissolved oxygen saturation, reaeration, CBOD decay, NBOD decay, sediment oxygen demand, photosynthesis, pH and alkalinity, nutrients, algae, zooplankton, and coliform bacteria. Factors affecting the specific phenomena and methods of measurement are discussed in addition to data on rate constants.

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Chapter 1

INTRODUCTION

1.1 BACKGROUND

The use of mathematical models to simulate ecological and water quality interactions in surface waters has grown dramatically over the past two decades. Simulation techniques offer an integrated and relatively sound course for evaluating wasteload abatement alternatives. Predictions of system behavior based upon mathematical simulation techniques may be misleading, however, particularly if the physical mechanisms involved are not accurately represented in the model. Furthermore, even where the model does faithfully describe mechanisms in the prototype, poor results may be obtained where insufficient data are available to estimate rate constants and coefficients.

Much of the work done in the water quality modeling field has been oriented toward improvement of models--toward incorporating better numerical solution techniques, toward an expanded complement of water quality constituents simulated, and toward realistic representations of modeled physical, chemical, and biological phenomena. There is, however, a need for a document that summarizes the rate constants and coefficients (e.g., nitrification rates and reaeration rates) needed in the models. This document is intended to satisfy that need.

The first edition of this document was published seven years ago (Zison et al., 1978). Because an extensive body of literature on rate constants and modeling formulations has emerged since that time, the United States Environmental Protection Agency has sponsored an updating of the manual. In addition, a workshop was held to evaluate the manual, to review the formulations and associated coefficients and rate values, and to provide further data for the final document. As a result of the literature review and workshop, a substantially new manual has been produced.

1.2 PURPOSE AND USE OF THIS MANUAL

This manual is intended for use by practitioners as a handbook--a convenient reference on modeling formulations, constants, and rates commonly used in surface water quality simulations. Guidance is provided in selecting appropriate formulations or values of rate constants for specific applications. The manual also provides a range of coefficient values that can be used to perform sensitivity analyses. Where appropriate, measurement techniques for rate constants are also discussed.

It was impossible, however, to encompass all formulations or to examine all recent reports containing rates data. It is hoped, therefore, that the user will recognize the desirability of seeking additional sources where questions remain about formulations or values. Data used from within this volume should be recognized as representing a sampling from a larger set of data. It should also be noted that there are often very real limitations involved in using literature values for rates rather than observed system values. It is hoped that this document will find its main use as a guide in the search for "the correct value" rather than as the sole source of that value.

1.3 SCOPE AND ARRANGEMENT OF MANUAL

In preparing this manual, an attempt was made to present a comprehensive set of formulations and associated constants. In contrast to the first edition (Zison et al.,1978), the manual has been divided into sections containing specific topics. Following this introduction, chapters are presented that discuss the following topics:

- Physical processes of dispersion and temperature
- Dissolved oxygen

- pH and alkalinity
- Nutrients
- Algae
- Zooplankton
- Coliforms

The parameters that are addressed in this manual are those that traditionally have been the focus of water quality management and the focus for control of conventional pollutants. These include temperature, dissolved oxygen, nutrients and eutrophication, and coliform bacteria. Higher organisms (fish, benthos) are not discussed, nor are the details of higher trophic levels in ecosystem models. Also, hydrodynamic processes, although important, are not dealt with in detail.

1.4 GENERAL OBSERVATIONS ON MODEL FORMULATIONS, RATE CONSTANTS, AND COEFFICIENTS

Each rate value or expression used in a model should not be chosen as an "afterthought", but should be considered as an integral part of the modeling process. A substantial portion of any modeling effort should go into selecting specific approaches and formulations based upon the objectives of modeling, the kinds and amounts of data available, and the strengths and weaknesses of the approach or formulation. Once formulations have been selected, a significant effort should be made to determine satisfactory values for parameters. Even where the parameter is to be chosen by calibration, it is clearly important to establish whether the calibrated value is within a reasonable range or not. Recent references on model calibration include Thomann (1983), National Council on Air and Stream Improvement (1982), and Beck (1983). Users should be aware that an acceptable model calibration does not imply that the model has predictive capability. The model may contain incorrect mechanisms, and agreement between model predictions and observations could have been obtained through an unrealistic choice of parameter values. Further, the future status of the prototype may be controlled by processes not even simulated in the model.

Values of many constants and coefficients are dependent upon the way they are used in modeling formulations. For example, while pollutant dispersion is an observable physical process, modeling this process is partly a mathematical construct. Therefore, constants that are used to represent the process (i.e., dispersion coefficients) cannot be chosen purely on the basis of physics since they also depend on the modeling approach. For example, to determine the dispersion coefficients in a model application to an estuary, both the time and length scales of the model must be considered. Whether the model is tidally averaged or simulates intra-tidal variations, and whether the model is 1-, 2-, or 3-dimensional, all influence the value of the appropriate dispersion coefficient for that model. Ford and Thornton (1979) discuss scale effects in ecological models, and conclude that inconsistent scales for the hydrodynamics, chemistry, and biology may produce erroneous model predictions.

Since coefficient values are never known with certainty, modelers are constantly faced with the question of how accurately rate constants should be known. The relationship between uncertainty in coefficient values and model predictions can be evaluated by performing sensitivity analyses. For models with few parameters, sensitivity analyses are generally straightforward. However, for complex models, sensitivity analyses are no longer straightforward since many dynamic interactions are involved. Sensitivity analyses are discussed in detail in Thornton and Lessem (1976), Thornton (1983), and Beck (1983).

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Chapter 2

PHYSICAL PROCESSES

2.1 INTRODUCTION

The purpose of this chapter is to give the reader an overview of how the major physical processes are incorporated into water quality and ecosystem simulations. Since a detailed review is beyond the scope of this report, the reader is encouraged to review the articles listed in Table 2-1 which represent several of the more complete and recent reviews of the state-of-the-art in physical process modeling.

Physical processes often simulated in water quality models include flow and circulation patterns, mixing and dispersion, water temperature, and the density distribution (which is a function of temperature, salinity, and suspended solids concentrations) over the water column. It is stressed that quality predictions are very dependent upon the physical processes and how well these are represented in the water quality simulations. Despite this dependence, the modeler often is forced to make a trade-off between acceptable degree of detail in water quality vs. physical process simulation due to cost or other restrictions. It is desirable from the standpoint of both the engineer and ecosystem analyst, therefore, to select the simplest model which satisfies the temporal and spatial resolution required for water quality and/or ecosystem simulation. For example, the optimum time step for dynamic simulation of a fully-mixed impoundment would be 3-6 hours for capturing diurnal fluctuations, and daily or weekly for strongly stratified impoundments which normally exhibit slowly varying conditions. In terms of spatial resolution required, the analyst should take advantage of the possible simplifications of dominate physical characteristics (i.e., physical shape, stratified layers, mixing zones, etc.).

TABLE 2-1. MAJOR REVIEWS OF MODELING STATE-OF-THE-ART

French, R.H. 1983. Lake Modeling: State-of-the-Art. In: CRC Critical Reviews in Environmental Control, Vol. 13, Issue 4, pgs. 311-357.
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2.1.1 Geometric Representation

2.1.1.1 Zero-Dimensional Models

Zero-dimensional models are used to estimate spatially averaged pollutant concentrations at minimum cost. These models predict a concentration field of the form $C = g(t)$, where t represents time. They cannot predict the fluid dynamics of a system, and the representation is usually such that an analytical solution is possible. As an example, the simplest representation of a lake is to consider it as a continuously stirred tank reactor (CSTR).

2.1.1.2 One-Dimensional Models

Most river models use a one-dimensional representation, where the system geometry is formulated conceptually as a linear network of segments or volume sections (see Figure 2-1). Variation of water quality parameters occur longitudinally (in the x-direction) as the water is transported out of one segment and into the next. The one-dimensional approach is also a popular method for simulation of small, deep lakes, where the vertical variation of temperature and other quality parameters is represented by a network of vertically stacked horizontal slices or volume segments.

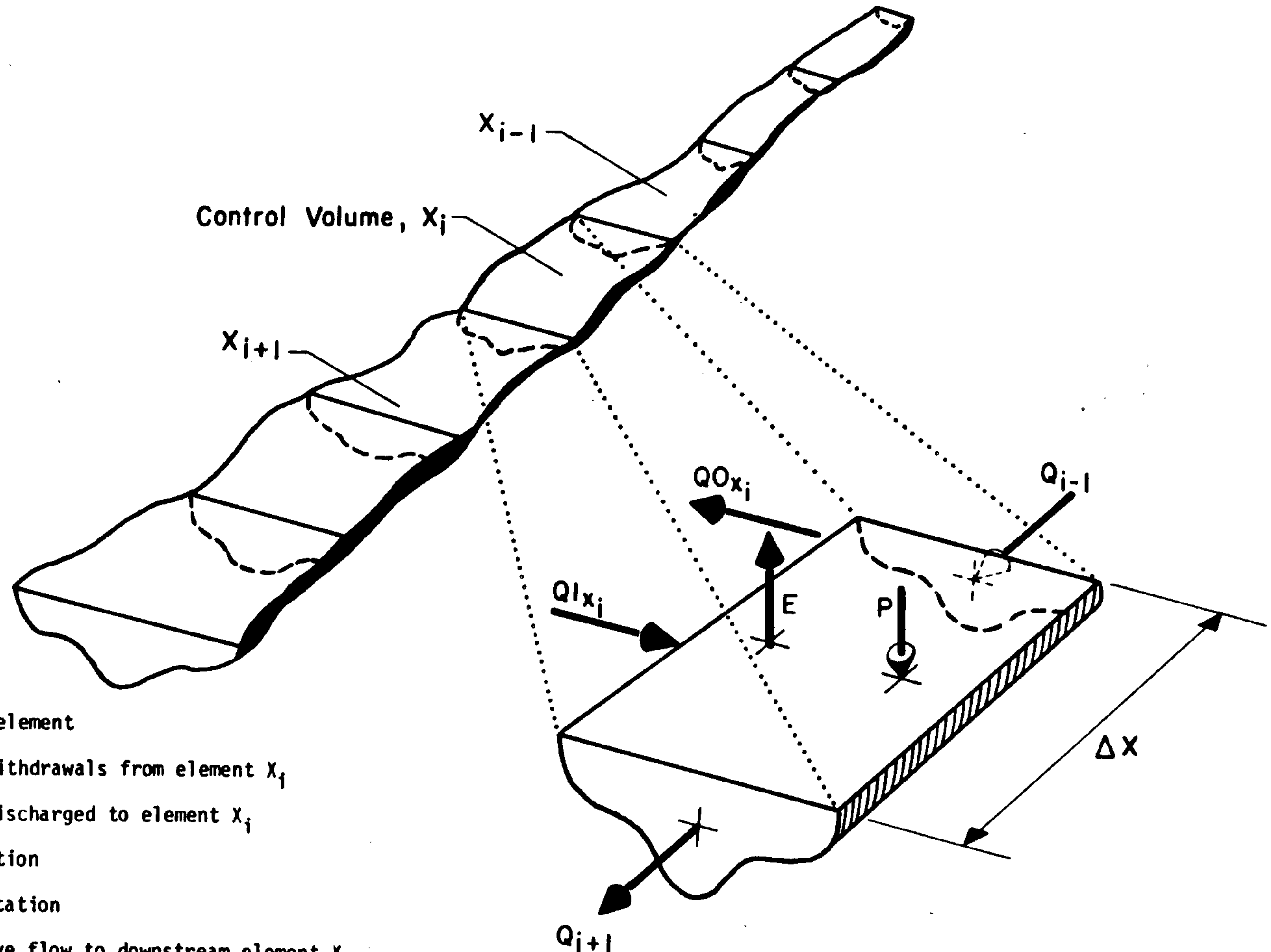
2.1.1.3 Multi-Dimensional Models

Water quality models of lakes and estuaries are often two- or three-dimensional in order to represent the spatial heterogeneity of the water bodies. Depending on the system, two-dimensional representations include a vertical dimension with longitudinal segmentation for deep and narrow lakes, reservoirs, or estuaries (Figure 2-2).

Three-dimensional spatial representations have been used to model overall lake circulation patterns. Part of the reason for this need is the concern with the water quality of the near-shore zone as well as deep zones of lakes. In addition, the different water quality interactions in these zones can lead to changes in the overall lake quality that cannot be predicted without this spatial definition.

2.1.2 Temporal Variation

Ecological models are distinguished on a temporal basis as being either "dynamic" or "steady-state". A strict steady-state assumption implies that the variables in the system equations do not change with time. Forcing functions, or exogenous variables, that describe environmental conditions which are unaffected by internal conditions of the system, have constant values. Inflows and outflows are discharged to and drawn from the system at



X_i = volume element

QO_{X_i} = water withdrawals from element X_i

QI_{X_i} = water discharged to element X_i

E = evaporation

P = precipitation

Q_{i+1} = advective flow to downstream element X_{i+1}

Q_{i-1} = advective flow from upstream element X_{i-1}

ΔX = longitudinal dimension of element

Figure 2-1. One-dimensional geometric representation for river systems (Chen and Wells, 1975).

a constant rate and any other hydrologic phenomena are also steady. Insolation, light intensity, photoperiods, extinction coefficients, and settling rates are a few examples of additional forcing functions which are held constant in a steady-state model. Constant forcing functions represent mean conditions observed in a system, and therefore the model cannot simulate cyclic phenomena.

A wide variety of planning problems can be analyzed by use of steady-state or quasi-steady (slowly varying) mathematical models which provide the necessary spatial detail for important water quality variables. Certain phenomena can achieve steady-state conditions within a short time interval and therefore can be modeled rather easily. Steady-state or quasi-steady representations are particularly useful because of their simplicity. Examples of phenomena which have been modeled on a steady-state basis are: 1) bacterial die-off, 2) dissolved oxygen concentrations (under certain conditions), and 3) nutrient distribution and recycle.

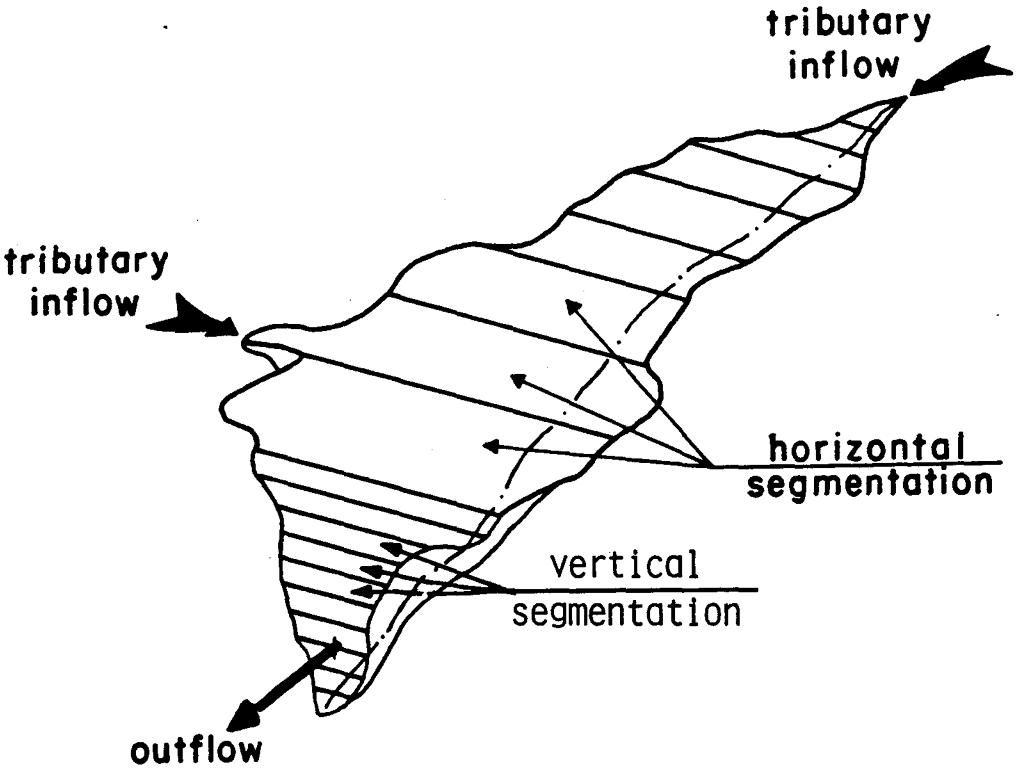


Figure 2-2. Two-dimensional geometric representation for lake systems (Baca and Arnett, 1976).

Many water quality or ecological models for rivers and lakes are concerned with the simulation of water quality variables that have substantial temporal variation and are linked to processes and variables that vary considerably. For example, the seasonal distribution of certain biological species and related abiotic substances may be of major importance. In these instances, dynamic models are required.

The process of selecting the correct time and length scales and then matching these with an appropriate model demands both an a priori understanding of the dominate physical, chemical and biological processes occurring within the system, as well as an understanding of a given model's theoretical basis and practical application limits. Proper guidance for model selection and application best comes from a thorough review of the relevant literature appropriate to the specific problem at hand. Ford and Thornton (1979), for example, present a detailed discussion of the time and length scales appropriate for the vertical one-dimensional modeling approach for reservoirs and lakes. The references presented in Table 2-1 as well as several others cited throughout this chapter discuss model compatibility requirements for various water body types and applications.

The remainder of this chapter focuses on advective transport, dispersive transport, and the surface heat budget.

2.2 ADVECTIVE TRANSPORT

The concentration of a substance at a particular site within a system is continually modified by the physical processes of advection and dispersion which transport fluid constituents from location to location. However, the total amount of a substance in a closed system remains constant unless it is modified by physical, chemical, or biological processes. Employing a Fickian type expression for turbulent mass flux, the three-dimensional advection-diffusion (mass balance) equation can be written as:

$$\frac{\partial c}{\partial t} + \frac{u\partial c}{\partial x} + \frac{v\partial c}{\partial y} + \frac{w\partial c}{\partial z} - \frac{\partial}{\partial x}\left(K_x \frac{\partial c}{\partial x}\right) - \frac{\partial}{\partial y}\left(K_y \frac{\partial c}{\partial y}\right) - \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right) = \Sigma S \quad (2\text{-}1)$$

where c = mean concentration of constituent, mass/volume

u = mean velocity in x-direction, length/time

v = mean velocity in y-direction, length/time

w = mean velocity in z-direction, length/time

K_x, K_y, K_z = eddy diffusion coefficients, $\text{length}^2/\text{time}$

ΣS = sum of source/sink rates, mass/(volume-time)

t = time

Difficulties exist in trying to correctly quantify the terms in this equation. The unsteady velocity field (u,v,w) is usually evaluated separately from Equation (2-1) so that the pollutant concentration, c, can be prescribed. The complete evaluation of the velocity field involves the simultaneous solution of the momentum, continuity, hydrostatic, and state equations in three dimensions (see Leendertse and Liu, 1975; Hinwood and Wallis, 1975). Although sophisticated hydrodynamic models are available, the detail and expense of applying such models are often not justified in water quality computations, especially for long term or steady-state simulations where only average flow values are required. For example, the annual thermal cycle for a strongly stratified reservoir with a relatively low inflow to volume ratio has been successfully simulated with only a crude one-dimensional, steady-state application of mass and energy conservation principles. On the other hand, simulation of large, weakly stratified impoundments dominated by wind driven circulation may require the ultimate, full representation of the unsteady velocity field in three dimensions.

The purpose of this section is to briefly familiarize the reader with the various types of approaches used to evaluate the velocity field in water quality models. Most hydrodynamic models internally calculate hydrodynamics with relatively little user control except for specification of forcing conditions such as wind, tides, inflows, outflows and bottom friction. Thus, the following paragraphs present only a summary discussion of the approaches used, organized according to the dimensional treatment of the model.

2.2.1 Empirical Specification of Advection

This is the crudest approach, in that the advective terms of the advection-diffusion equation (Equation 2-1) are directly specified from field data. Empirical specification is quite common in water quality models for rivers, but is also often used in steady-state or slowly-varying estuary water quality models (e.g., O'Connor et al. (1973)). In these types of estuary models, specification of the dispersion coefficients is critical since dispersion must account for the mixing which in reality is caused by the oscillatory tidal action. Due to the highly empirical treatment of the physical processes in such models, the model "predictions" remain valid for only those conditions measured in the field. These models cannot predict water quality variations under other conditions, thus increasing the demand on field data requirements. Examples of models representative of the above approach include O'Connor et al. (1973) and Tetra Tech (1977).

2.2.2 Zero Dimensional Models for Lakes

A coarse representation of the water system as a continuously stirred tank reactor (CSTR) is often sufficient for problem applications to some lakes where detailed hydrodynamics are not required. Since in this zero-dimensional type of representation there is only a single element, no transport direction can be specified. The quantity of flow entering and leaving the system alone determines water volume changes within the element. Examples of zero-dimensional models include lake models by Anderson et al. (1976).

2.2.3 One-Dimensional Models for Lakes

For lake systems with long residence times and stratification in the vertical direction, vertical one-dimensional representations are common. Horizontal layers are imposed and advective transport is assumed to occur only in the vertical direction.

Generally the tributary inflows and outflows are assumed to enter and leave the lake at water levels of equal density. Since water is essentially incompressible the inflow is assumed to generate vertical advective flow (via the continuity equation) between all elements above the level of entry. The elements below this level, containing higher density water, are assumed to be unaffected. Examples of one-dimensional lake models include Lombardo (1972, 1973), Baca et al. (1974), Chen and Orlob (1975), Thomann et al. (1975), Imberger et al. (1977), HEC (1974), Markofsky and Harleman (1973), and CE-QUAL-R1 (1982).

For lake or reservoir systems exhibiting complex horizontal interflows, inflows, and outflows, semi-empirical formulations have been developed to distribute inflows and to determine the vertical location from which outflows arise, depending on stratification conditions. Examples include models by U.S. Army Corps of Engineers (1974), Baca et al. (1976), and Tetra Tech (1976).

2.2.4 One-Dimensional Models for Rivers

Most river models represent river systems conceptually as horizontal linear networks of segments or volume elements. The process of advection is assumed to transport a constituent horizontally by movement of the parcel of water containing the constituent. In general, there are two approaches to treat the advection in river models. One approach requires field calibration of the river flow properties by measuring flows and cross sectional geometry at each model segment over a range of flow magnitudes. A power series can then be developed for each cross section to interpolate or extrapolate for other flow events. Such an approach is especially appropriate for rivers exhibiting complex hydraulic properties (i.e., supercritical flows, cascades, etc.) and when steady state solutions are of interest. Examples of such models include Tetra Tech (1977).

A second, more rigorous approach for simulating river advection involves the simultaneous solution of the continuity and momentum equations for the portion of the river under study. This approach is considered more "predictive" than the former since empirical flow data are required only for model calibration and verification. It is also more accurate and appropriate for use in transient water quality simulations. In either case, however, geometrical data on the cross-sectional shapes of the river are required. Examples of models representative of the latter approach include Brocard and Harleman (1976), and Peterson et al. (1973).

2.2.5 One-Dimensional and Pseudo-Two-Dimensional Models for Estuaries

A natural extension of the one-dimensional river model has been to estuary systems, either as a one-dimensional representation for narrow estuaries or as a system of multiple interconnecting one-dimensional channels for pseudo-representation of wider or multi-channeled estuaries. In either case, advection is determined through the simultaneous solution of the continuity and momentum equations together with appropriate tidal boundary conditions. These types of models are generally quite flexible in their ability to handle multiple inflows, transient boundary conditions, and complex geometrical configurations. Two primary approaches include the "link-node" network models by Water Resources Engineers (WRE) (1972), and the finite element model (Galerkin Method) by Harleman et al. (1977).

2.2.6 Two-Dimensional Vertically Averaged Models for Lakes and Estuaries

Vertically averaged, two-dimensional models have proven to be quite useful, especially in modeling the hydrodynamics and water quality of relatively shallow estuaries and wind-driven lakes. The crucial assumption of these models is the vertically well-mixed layer that allows for vertical integration of the continuity, momentum, and mass-transport equations. Such models are frequently employed to provide the horizontal advection for water quality models since they are relatively inexpensive to operate compared to the alternatives of large scale field measurement programs or fully three-dimensional model treatments. There exist well over fifty models which would fit into the two-dimensional, vertically averaged classification. Examples of models that have been widely used and publicized include Wang and Connor (1975), Leendertse (1970), Taylor and Pagenkopf (1980), and Simons (1976).

2.2.7 Two-Dimensional Laterally Averaged Models for Reservoirs and Estuaries

In recent years, laterally averaged models have become standard simulation techniques for reservoirs or estuaries which exhibit significant vertical and longitudinal variations in density and water quality conditions. The two-dimensional laterally averaged models require the assumption of uniform lateral mixing in the cross channel direction. Although this simplification eliminates one horizontal dimension, the solution of the motion equations in the remaining longitudinal and vertical dimensions requires a much more rigorous approach than for the two-dimensional vertically averaged models. In order to correctly simulate the vertical effects of density gradients on the hydrodynamics and mass transport, both the motion (continuity and momentum) and advective-diffusion equations must be solved simultaneously. In addition, such models must also treat the vertical eddy viscosity (momentum transfer due to velocity gradients) and eddy diffusivity (mass transfer due to concentration gradients) coefficients, which are directly related to the degree of internal mixing and the density structure over the water column. Mathematical treatment of vertical diffusion and vertical momentum transfer varies greatly between models, and will be discussed further in this document. Examples of laterally averaged reservoir models include Edinger and Buchak (1979) and Norton et al. (1973). Examples of laterally averaged models developed for estuaries include Blumberg (1977), Najarian et al. (1982) and Wang (1979).

2.2.8 Three-dimensional Models for Lakes and Estuaries

Fully three-dimensional and layered models have been the subject of considerable attention over the last decade. Although still a developing field, there are a number of models which have been applied to estuary, ocean, and lake systems with moderate success. As with laterally averaged two-dimensional models, the main technical difficulty in this approach is in the specification of the internal turbulent momentum transfer and mass diffusivities, which are ideally calibrated with field observations, thus making availability of adequate prototype data an important consideration. An additional factor of great importance is the relatively large computation cost of running three-dimensional models, especially for long-term water quality simulations. In many cases, the effort and cost of running such models is difficult to justify from purely a water quality standpoint. However, as computational costs continue to decrease and sophistication of numerical techniques increases, such models will eventually play an important role in supplying the large scale hydrodynamic regimes in water quality simulations. Examples of the more prominent three-dimensional models include Blumberg and Mellor (1978), Leendertse and Liu (1975), Sheng and Butler (1982), Simons (1976) and King (1982).

2.3 DISPERSIVE TRANSPORT

2.3.1 Introduction

The purpose of this section is to show how dispersive transport terms are incorporated into the equations of motion and continuity by temporal and spatial averaging (a detailed discussion of this subject is also given by Fischer et al. (1979)). A consequence of temporal averaging of either instantaneous velocity or concentration is to produce a smoothed velocity or concentration response curve over time. Figure 2-3 illustrates both instantaneous velocity and time-smoothed curves. The velocities V and $\overline{V}$ are related by

$$V = \overline{V} + V' \qquad (2\text{-}2)$$

where V = instantaneous velocity, length/time
$\overline{V}$ = time-smoothed velocity, length/time
V' = velocity deviation from the time-smoothed velocity, length/time

The velocity component V' is a random component of velocity which vanishes when averaged over the appropriate time interval (i.e., $\overline{V'} = 0$).

By averaging, the stochastic components are removed from the momentum and mass conservation equations. However, cross product terms appear in the equations, such as $\overline{V'_x V'_x}$ and $\overline{V'_x V'_y}$ in the case of the momentum equation, and $\overline{V'_x C'}$ and $\overline{V'_y C'}$ in the case of the mass conservation equation (where C' is the instantaneous concentration fluctuation, and V'_x and V'_y are the random velocity deviations in the x and y directions, respectively). In the case of the momentum equation these terms are called turbulent momentum fluxes, and in the case of the mass conservation equation they are called turbulent mass fluxes. It is through these terms that eddy viscosity and eddy diffusivity enter into the momentum and mass conservation equations.

To solve the time-smoothed equations, the time averaged cross product terms are expressed as functions of time averaged variables. Numerous empirical expressions have been developed to do this. The expressions most often applied are analogous to Newton's law of viscosity in the case of turbulent momentum transport and Fick's law of diffusion in the case of turbulent mass transfer. Expressed quantitatively these relationships are of the form:

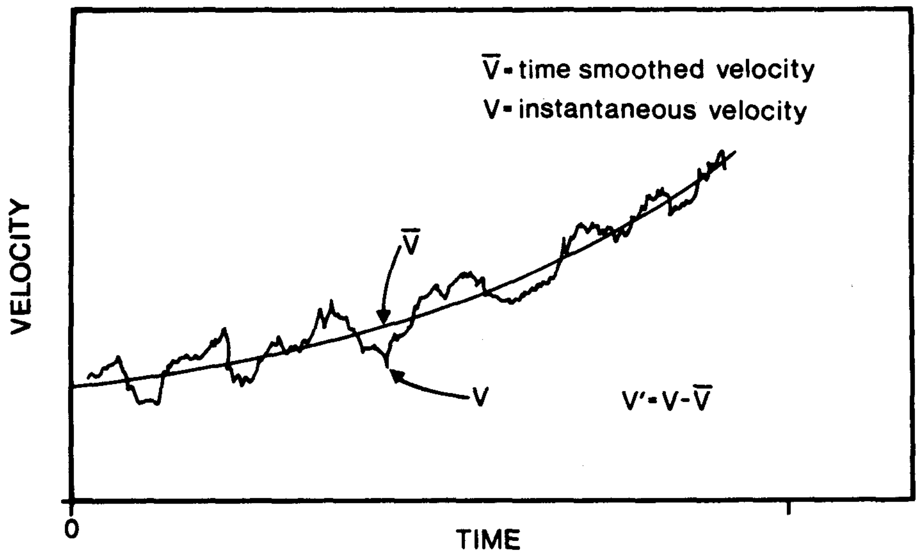


Figure 2-3. Oscillation of velocity component about a mean value (redrawn after Bird et al., 1960).

$$\overline{\rho V'_x V'_y} = E \frac{\partial \overline{V}_x}{\partial y} \tag{2-3}$$

$$\overline{V'_y C'} = K \frac{\partial \overline{C}}{\partial y} \tag{2-4}$$

where E = eddy viscosity, mass/(length-time)

K = eddy diffusivity, length^2/time

$\overline{V}_x$ = time smoothed velocity in the x direction, length/time

$\overline{C}$ = time smoothed concentration, mass/volume

ρ = mass density, mass/volume

In natural water bodies the turbulent viscosity and diffusivity given by Equations (2-3) and (2-4) swamp their counterparts on the molecular level. The relative magnitude between eddy diffusivities and molecular diffusion coefficients is depicted graphically in Figure 2-4.

In addition to temporal averaging, spatial averaging is often used to simplify three dimensional models to two or one dimensions. As an illustration consider the vertically averaged mass transport equation. Before averaging, the governing three dimensional mass transport equation is typically written as:

$$\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} + \frac{\partial (vc)}{\partial y} + \frac{\partial (wc)}{\partial z} = -\frac{\partial}{\partial x}(Q_x) - \frac{\partial}{\partial y}(Q_y) - \frac{\partial}{\partial z}(Q_z) \tag{2-5}$$

where c = the local (time smoothed) concentration, mass/volume

u,v,w = the local (time smoothed) water velocities, length/time

Q_x, Q_y, Q_z = the local diffusive fluxes, mass/(length^2-time)

Before spatial averaging, the local concentration and velocities can be expressed by a vertically averaged term and a deviation term:

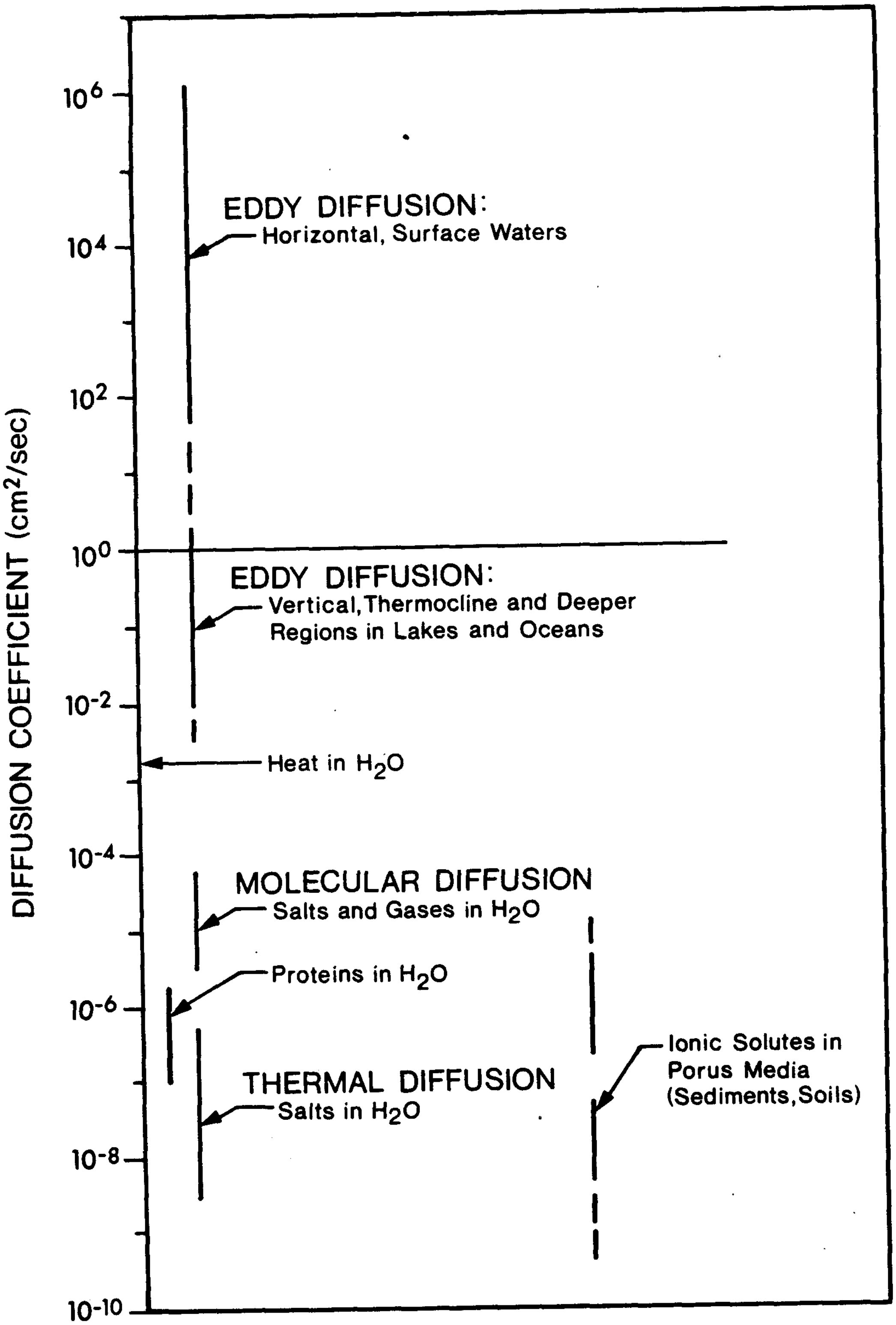


Figure 2-4. Diffusion coefficients characteristic of various environments (redrawn after Lerman, 1971).

$$c = c_h + c_h'$$
$$u = u_h + u_h'$$
$$v = v_h + v_h' \qquad (2\text{-}6)$$

where c,u,v = previously defined

c_h = vertically averaged concentration, mass/volume

$$= \frac{1}{h} \int_0^h c\,dz \qquad (2\text{-}7)$$

c_h' = deviation from c_h at any point in the water column, mass/volume

u_h, v_h = vertically averaged water velocities, length/time

$$= \int_0^h u\,dz, \quad \int_0^h v\,dz \qquad (2\text{-}8)$$

u_h', v_h' = deviation from u_h, v_h at any point in the water column, length/time

h = local water depth, length

Equation (2-5) can now be written in its vertically averaged form:

$$\frac{\partial c_h}{\partial t} + \frac{\partial(u_h c_h)}{\partial x} + \frac{\partial(v_h c_h)}{\partial y} = -\frac{\partial}{\partial x}\int_0^h (Q_x + u_h' c_h')\,dz - \frac{\partial}{\partial y}\int_0^h (Q_y + v_h' c_h')\,dz \qquad (2\text{-}9)$$

It is noted that when vertical integration is performed on the three-dimensional mass conservation equation, cross product terms appear in the resulting two-dimensional equation, just as they do when temporal averaging is done because vertical gradients generally exist in both the concentration and velocity fields. The horizontal turbulent diffusion fluxes Q_x, Q_y are usually expressed in terms of the gradients of the vertically averaged concentration and the turbulent diffusion coefficient, which in general form are written:

$$Q_x = -\varepsilon_{xx} \frac{\partial c_h}{\partial x} - \varepsilon_{xy} \frac{\partial c_h}{\partial y} \tag{2-10a}$$

$$Q_y = -\varepsilon_{yx} \frac{\partial c_h}{\partial x} - \varepsilon_{yy} \frac{\partial c_h}{\partial y} \tag{2-10b}$$

where ε_{xx}, ε_{xy}, ε_{yx}, ε_{yy} = turbulent eddy diffusion coefficients

By analogy, the horizontal transport terms, $u_h' c_h'$ and $v_h' c_h'$, associated with vertical velocity variations (i.e., differential advection), are expressed by means of the shear dispersion coefficients:

$$u_h' c_h' = -E^d_{xx} \frac{\partial c_h}{\partial x} - E^d_{xy} \frac{\partial c_h}{\partial y} \tag{2-11a}$$

$$v_h' c_h' = -E^d_{yx} \frac{\partial c_h}{\partial x} - E^d_{yy} \frac{\partial c_h}{\partial y} \tag{2-11b}$$

where $E^d_{xx}, E^d_{xy}, E^d_{yx}, E^d_{yy}$ = shear dispersion coefficients

By combining Equations (2-10) and (2-11), the final form of the vertically averaged mass transport equation can be written as:

$$\frac{\partial c_h}{\partial t} + \frac{\partial (u_h c_h)}{\partial x} + \frac{\partial (v_h c_h)}{\partial y} = \frac{\partial}{\partial x}\left(D_{xx} h \frac{\partial c_h}{\partial x} + D_{xy} h \frac{\partial c_h}{\partial y}\right)$$

$$\frac{\partial}{\partial y}\left(D_{xy} h \frac{\partial c_h}{\partial x} + D_{yy} h \frac{\partial c_h}{\partial y}\right) \tag{2-12}$$

where D_{xx}, D_{xy}, D_{yy} = dispersion coefficients which account for mass transport due to both concentration and velocity gradients over the vertical.

One-dimensional mass conservation equations result when a second spatial averaging is performed. The one-dimensional equations express changes along the main flow axis. As expected, the diffusion terms are again different from their two-dimensional counterparts. Consequently, the type and magnitude of the diffusion terms appearing in the simulation equations depends not only on the water body characteristics, but the model used to simulate the water body.

2.3.2 Vertical Dispersive Transport

Vertical dispersive transport of momentum and mass becomes important in lakes or estuaries characterized by moderate to great depths. In a lake environment, vertical mixing is generally caused by wind action on the surface through which eddy turbulence is transmitted to the deeper layers by the action of shear stresses. In estuaries, typically the vertical mixing is induced by the internal turbulence driven by the tidal flows, in addition to surface wind effects. Similarly, the internal mixing in deep reservoirs is primarily caused by the flow-through action. In each environment, however, the amount of vertical mixing is controlled, to a large extent, by the degree of density stratification in the water body.

Treatment of vertical mixing processes in mathematical models is generally achieved through the specification of vertical eddy viscosity (E_v) and eddy diffusivity (K_v) terms, as previously discussed. As observed by McCutcheon (1983), however, there is little consensus on what values the vertical eddy coefficients should have and how eddy viscosity and eddy diffusivity are related. At present, the procedure for estimating these coefficients is generally limited to empirical techniques that range from specifying a constant E_v and K_v to relating to some measure of stability, i.e., the Richardson number Ri. In this approach, the ratio of the coefficients for stratified flow to the coefficients for unstratified flow is expressed as a function of stability f(s):

$$E_v/E_{vo} = f_1(s), \tag{2-13}$$

$$K_v/K_{vo} = f_2(s), \tag{2-14}$$

and $$E_{vo} = Pr\ K_{vo} \tag{2-15}$$

where $E_{vo} = kzu_*(1 - z/h)$ for shear layers and Pr = the Prandtl or Schmidt number, which is generally close to unity for open-channel shear flow (Watanabe et al., 1984).

In addition

k = von Karman's constant (~0.4), dimensionless
z = distance above the bottom, length
u_* = shear velocity, length/time
h = depth of flow, length

A widely used formula which relates E_v/E_{vo} to stability involves the Munk and Anderson (1948) formulation (as reported by McCutcheon (1983)):

$$E_v/E_{vo} = (1 + 10\ Ri)^{-1/2} \qquad (2\text{-}16)$$

and

$$K_v/K_{vo} = (1 + 3.33\ Ri)^{-3/2} \qquad (2\text{-}17)$$

where $Ri = \frac{g}{\rho}\frac{\partial\rho}{\partial z}\Big/\left(\frac{\partial u}{\partial z}\right)^2$, dimensionless (2-18)

ρ = density, mass/volume
u = the mean horizontal velocity at a point z above the bottom, length/time
g = acceleration of gravity, length/time^2

As reported by McCutcheon (1983), in a recent review of available data for stratified water flows (Delft, 1979) Equations (2-16) and (2-17) were found to fit the data better than several other similar formulations. Models by Waldrop (1978), Harper and Waldrop (1981), Edinger and Buchak (1979), O'Connor and Lung (1981), Najarian et al. (1982), and Heinrich, Lick and Paul (1981) use this scheme. In some models, the coefficients and exponents in Equation (2-16) and (2-17) are not adjusted, and any discrepancies between field measurements and model predictions are attributed to the inexactness of the model. In other models, the coefficients and exponents are calibrated on a site specific basis.

For model simulations of mixing through and below the thermocline, the Munk and Anderson type formulas appear to be less adequate (McCutcheon, 1983). Odd and Rodger (1978) developed site specific eddy viscosity formulations for the Great Ouse Estuary in Britain:

$$E_v/E_{vo} = (1 + bRi)^{-n} \quad \text{for } Ri \leq 1 \tag{2-19}$$

and

$$E_v/E_{vo} = (1 + b)^{-n} \quad \text{for } Ri > 1 \tag{2-20}$$

where b and n are coefficients. The depth varying Ri is used if Ri increases continuously starting at the bed and extending over 75 percent or more of the depth. Where a significant peak in Ri occurs in the vertical gradient, that peak Ri is used for all depths in the equation above. McCormick and Scavia (1981) make a correction for K_v in Lake Ontario and Lake Washington studies that is similar to corrections of E_v by Odd and Rodger. Above the hypolimnion, they apply a modification of the Kent and Pritchard (1959) equation:

$$K_v = u_* / \beta R_o \tag{2-21}$$

where $R_o = -kz^2 \frac{g}{\rho} \frac{\partial \rho}{\partial z} / u_*^2$ (2-22)

β = constant

Below the thermocline a constant K_v was specified for Lake Ontario. In Lake Washington, Equation (2-21) and (2-22) were applied throughout the depth. In Lake Washington bottom shear was important for mixing as opposed to deeper Lake Ontario where surface wind shear dominated the mixing process.

Several other formulations for E_v and K_v have been developed which are not based on the Munk and Anderson equations. For example, Blumberg (1977), in his laterally averaged model of the Potomac River Estuary, employed an expression for K_v which uses a ratio of Ri to a critical Ri to relate K_v to stability, where:

$$K_v = K_1^2 z^2 \left(\frac{1-z}{h}\right)^2 \left|\frac{u}{z}\right| \left(1- \frac{Ri}{Ri_c}\right)^{1/2} \qquad (2\text{-}23)$$

where K_1 is a turbulence constant which must be determined by calibration, and Ri_c is the critical Richardson number, which is the value of Ri at which mixing ceases due to strong stratification. Blumberg also related E_v to K_v through the following formulation:

$$E_v = K_v\ (1 + Ri) \qquad \text{for } 0 < Ri < Ri_c \qquad (2\text{-}24a)$$

$$E_v = K_v = 0 \qquad \text{for } Ri \geq Ri_c \qquad (2\text{-}24b)$$

Using the above formulations, Blumberg obtained reasonably good comparisons for salinity distributions in the Potomac River.

Simons (1973) based his formulation for K_v for Lake Ontario on the results of dye diffusion experiments performed by Kullenberg et al. (1973) where K_v is expressed as:

$$K_v = C \frac{W^2}{N^2} \left|\frac{\partial q}{\partial z}\right| \qquad (2\text{-}25)$$

where C = an empirical constant, $(2 \sim 8)10^{-8}$

W = wind speed, length/time

N^2 = Brunt-Väisälä frequency, $\frac{g}{\rho}\frac{\partial \rho}{\partial z}$, time^{-2}

$\frac{\partial q}{\partial z}$ = vertical shear of the current, time^{-1}

Simons also assumed that the vertical eddy viscosity coefficient was based on a similar relationship.

The above formulation is a result of experiments performed in fjords, coastal and open sea areas, as well as from Lake Ontario, and is generally valid for expressing the vertical mixing in the upper 20 m for persistent winds above 4-5 m/sec. The lower value of the numerical constant refers to the lake data and the higher value to the oceanic data.

For low and varying wind speeds Equation (2-25) will not be valid (Murthy and Okubo, 1975). In these cases the internal mixing is considered to be governed by local processes, i.e., the energy source is the kinetic energy fluctuations. Kullenberg (as reported by Murthy and Okubo (1975)) proposed the following relation for weak local winds:

$$K_v = 4.1 \times 10^{-4} \, q'^2 (N^2)^{-1} \left| \frac{\partial q}{\partial z} \right| \tag{2-26}$$

where $q'^2 \equiv V_x'^2 + V_y'^2$

V_x', V_y' = velocity fluctuations in the x and y directions, respectively, length/time

Equation (2-26) is representative of the vertical mixing both above and below the thermocline under conditions of low wind speeds.

Tetra Tech (1975) has used the following empirical expressions for computation of the vertical eddy thermal diffusivity, K_v, in their three-dimensional hydrodynamic simulation of Lake Ontario.

$$K_v = 100 \frac{|\tau_s|}{\rho_o} \left(\frac{3}{1+3.3Ri} \right)^{1/2} \tag{2-27}$$

where ρ_o = density of fresh water at 4^oC, mass/volume

τ_s = surface wind stress, mass/(length-time^2).

Lake systems that are represented geometrically as a series of completely mixed horizontal slices consider advective and dispersive transport processes to occur in the vertical direction alone. Baca and Arnett (1976), in their one-dimensional hydrothermal lake model, proposed the following expression for determining the one-dimensional vertical dispersion coefficient:

$$K_v = a_1 + a_2 \, V_w \, d^{-4.6z/d} \tag{2-28}$$

where K_v = vertical dispersion coefficient, m^2/sec

z = depth, m

V_w = wind speed, m/sec

d = depth of thermocline, m

a_1, a_2 = empirical constants, m^2/sec and m respectively

The following table of values (Table 2-2) for a_1 and a_2, as given by Baca and Arnett (1976), were obtained from previous model applications.

TABLE 2-2. VALUES FOR EMPIRICAL COEFFICIENTS a_1 and a_2

Lake	Description	Max. Depth (m)	a_1 (m^2/sec)	a_2 (m)
American Falls	well-mixed	18	1×10^{-5}	1×10^{-4}
Lake Washington	stratified	65	1×10^{-6}	1×10^{-5}
Lake Mendota	stratified	24	5×10^{-7}	5×10^{-5}
Lake Wingra	well-mixed	5	5×10^{-5}	2×10^{-4}
Long Lake	linearly stratified	54	5×10^{-6}	5×10^{-5}

The vertical eddy viscosity and eddy diffusivity concepts continue to be practical and are a popular means for simplifications of the momentum and mass conservation equations. As pointed out by Sheng and Butler (1982) and McCutcheon (1983), however, a wide variety exists among the various forms of the vertical turbulence stability functions determined empirically by various investigators, and suggest that the appropriate stability function is dependent on the type of numerical scheme used and the nature of the water body under study. The wide variation in formulations is, in part, due to the attempt to fit empirical functions determined under specific field conditions to a wider range of water body types and internal mixing phenomena. Due to the possibility of applying an empirical relationship beyond its valid limits, site-specific testing of formulations for E_v and K_v will probably be required in most model applications.

The above discussion has concentrated on the eddy diffusion concept on which many models are based. However, an alternative to this approach is the mixed layer concept which has been successfully applied by numerous investigators to predict the vertical temperature regime of lakes and reservoirs. As summarized by Harleman (1982), the mixed layer or integral energy concept involves the following: the turbulent kinetic energy (TKE) generated by the surface wind stress is transported downward and acts to mix the upper water column layer. At the interface between the upper mixed layer and the lower quiescent layer, the remaining TKE, plus any that may be locally generated by interfacial shear (minus dissipation effects), is transferred into potential energy by entraining quiescent fluid from below the interface into the mixed layer. This entrainment, in addition to any vertical advective flows, determines the thickness of the mixed layer. TKE is also produced by convective currents which occur during periods of cooling, and can contribute to the mixing process. Also, the total vertical heat balance due to surface heat flux and internal absorption must be considered in evaluating the vertical density distribution and potential energy of the water column. A discussion of the mixed layer model approach can be found in Harleman (1982), French (1983) and Ford and Stefan (1980). Models based on this approach include those by Stefan and Ford (1980), Hurley-Octavio et al. (1977), Imberger et al. (1977) and CE-QUAL-R1 (1982).

2.3.3 Horizontal Eddy Diffusive Transport

Generally, horizontal eddy diffusivity is several orders of magnitude greater than the vertical eddy diffusivity (see Figure 2-4). The Journal of the Fisheries Research Board of Canada (Lam and Jacquet, 1976) reported a range of values for the horizontal diffusivity in lakes from 10^4 to 10^6 cm^2/sec. Unlike diffusive transport in open-channel type flows, diffusion in open water, such as in lakes and oceanic regimes, cannot be effectively related to the mean flow characteristics (Watanabe et al., 1984). Oceanic or lake turbulence represents a spectrum of different eddies resulting from the breakdown of large-scale circulations in shore zones and by wind and wave induced circulations. Attempts to analyze this phenomenon have demonstrated that the horizontal diffusive transport, D_h depends on the length scale L of the phenomenon. The most widely used formula is the four-thirds power law:

$$D_h = A_D L^{4/3} \tag{2-29}$$

where A_D is the dissipation parameter (of the order .005, with D_h in cm^2/sec). The length scale L is loosely defined depending on the nature of the diffusion phenomenon. For a waste discharge in the ocean, for example, L is often estimated based on the diffuser length, which is typically the order of a kilometer. Another example is to estimate L based on the length of the tidal excursion in estuaries or coastal areas. When using Equation (2-29) to estimate the diffusion coefficient in two or three-dimensional numerical models, the length scale is often taken as the size of the horizontal grid spacing, since this approximates the minimum scale of eddies which can be reproduced in the model.

Useful summaries of lake and ocean diffusion data are given by Yudelson (1967), Okubo (1968) and Osmidov (1968). Okubo and Osmidov (1970) have graphed the empirical relationship between the horizontal eddy diffusivity and the length scale, as shown in Figure 2-5. According to Figure 2-5:

$$D_h \approx 2 \times 10^{-3} L^{4/3} \quad \text{for } L < 10^5 \text{cm}$$

$$D_h \approx 10^4 \quad \text{for } 10^5 < L < 5 \times 10^5 \text{ cm}$$

$$D_h \approx 10^{-3} L^{4/3} \quad \text{for } L > 5 \times 10^5 \text{ cm} \tag{2-30}$$

where D_h is in cm^2/sec and L in cm. Based on these empirical observations, it is seen that the dissipation parameter of the four-thirds law decreases at larger length scales.

A comprehensive collection of diffusion data in the ocean was presented by Okubo (1971), who proposed as best fit to all the data the relation:

$$D_h = 0.01L^{1.15} \qquad \text{for } 10^3 \leq L \leq 10^8 \text{ cm} \qquad (2\text{-}31)$$

which is graphed in Figure 2-6. According to Christodoulou et al. (1976), the four-thirds law seems theoretically and experimentally acceptable for expressing the horizontal eddy diffusivity in large lakes and in the ocean, providing the length scales of interest are not of the order of the size of the energy containing eddies. In addition, the four-thirds law is not fully acceptable near the shore, due to the shoreline and bottom interference.

Two examples of the use of Equation (2-29) in lake models are in Lam and Jacquet (1976) and Lick et al. (1976). Lam and Jacquet obtained the following formulation for the horizontal eddy diffusivity for lakes, based on experimental results:

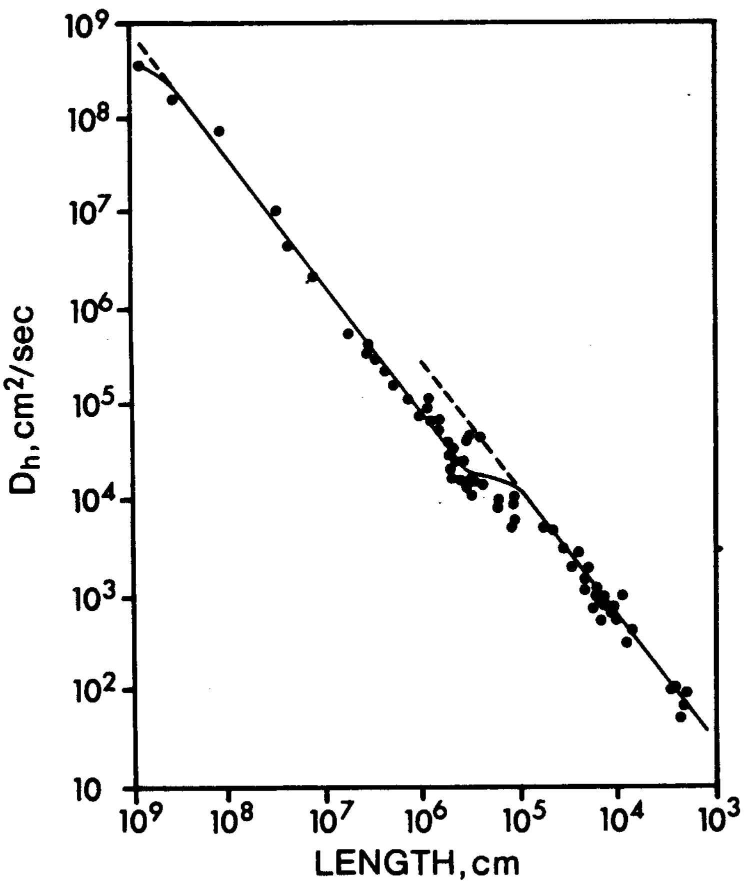


Figure 2-5. Dependence of the horizontal diffusion coefficient on the scale of the phenomenon (after Okubo and Osmidov (1970)).

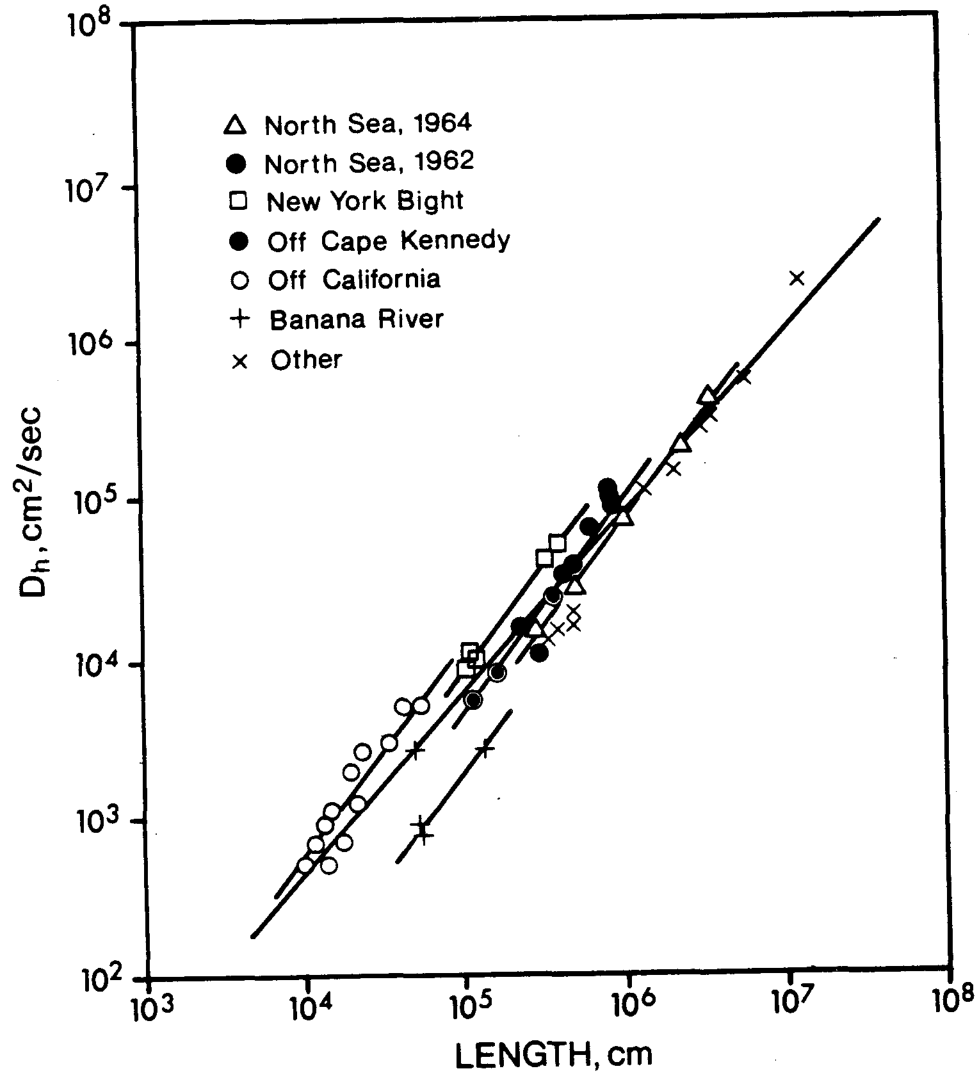


Figure 2-6. Okubo's diffusion data and 4/3 power lines (after Okubo (1971)).

$$D_h = .0056L^{1.3} \qquad (2\text{-}32)$$

where D_h = horizontal eddy diffusivity, cm^2/sec
L = length scale of grid, cm

As reported by Lam and Jacquet, for a grid size larger than 20 km, the diffusivity is expected to be essentially constant (10^6 cm^2/sec).

Lick (1976) used a similar formulation after Osmidov (1968), Stommel (1949), Orlob (1959), Okubo (1971) and Csanady (1973):

$$D_h = a\ E^{1/3}\ L^{4/3} \tag{2-33}$$

where a = constant of proportionality, of the order 0.1
E = rate of energy dissipation per unit mass

Observations by Lick indicated values of 10^4 to 10^5 cm^2/sec for D_h for the overall circulation in the Great Lakes with smaller values indicated in the near-shore regions.

The above relationships can be used as a general guide to evaluate the horizontal diffusivities in a numerical model, where the grid size may be regarded as the approximate length scale of diffusion. However, as pointed out by Murthy and Okubo (1977): (1) the data upon which these empirical relations are obtained do not represent diffusion under severe weather conditions, and thus may include a bias towards relatively mild conditions; (2) the horizontal diffusivity can vary (depending primarily upon the environmental conditions) by an order of magnitude for the same length scale of diffusion; (3) the definition of the length scale of diffusion for the horizontal diffusivity is somewhat arbitrary; and (4) the horizontal diffusivity varies by an order of magnitude between the upper and lower layers of oceans and deep lakes. Thus, to develop reliable three-dimensional models the scale and stability dependence of eddy diffusivities and the large variability of the magnitude of the eddy diffusivity with depth and environmental factors (wind, waves, inflows, etc.) must somehow be incorporated into the models.

The formulations for horizontal eddy diffusivity discussed above are generally representative of empirical (physical) diffusion behavior and are most compatible with a three-dimensional approach. As previously discussed, horizontal dispersion is the "effective diffusion" that occurs in two-dimensional mass transport equations that have been integrated over the depth. Thus the horizontal dispersion must account for both horizontal eddy diffusivity due to horizontal turbulence and concentration gradients, as well as the effective spreading caused by velocity and concentration variations over the vertical. In addition, any simplifications in the velocity field used in modeling must also be accounted for in the dispersion coefficients. The less detailed the flow field is modeled, the larger the dispersion coefficient needs to be to provide for the spreading that would occur under the actual circulation (Christodoulou and Pearce, 1975). Therefore, the dispersion coefficients are characteristic not only of the flow conditions to be simulated, but more significantly of the way the process is modeled. Hence these coefficients are model-dependent and difficult to quantify in any general, theoretical manner. For example, many two-dimensional models use a constant dispersion coefficient over the whole model domain as well as over time despite the fact that dispersion changes both spatially and temporally as the circulation features change. An example of a model that uses constant dispersion coefficients is Christodoulou et al. (1976).

One two-dimensional model which utilizes variable dispersion coefficients (velocity dependent) in time and space is the finite difference model by Taylor and Pagenkopf (1981). They utilize Elder's (1959) relationship for anisotropic flow where the dispersion of a substance is proportional to the friction velocity, u_*, and the water depth, h, as follows:

$$D_r = 5.9\ u_* h \tag{2-34}$$

$$D_n = 0.2\ u_* h \tag{2-35}$$

where D_r = dispersion coefficient along the flow axis, length^2/time

D_n = dispersion coefficient normal to the flow axis, length^2/time

u_* = $\sqrt{\frac{f}{8}}\ |\vec{U}|$, length/time

f = Darcy-Weisbach friction factor, dimensionless

$|\vec{U}|$ = absolute value of mean velocity along flow axis, length/time

The above relationship is incorporated into the two dimensional mass conservation equation resulting in an anisotropic mixing process which calculates a dispersion coefficient at each time step and node as a function of the instantaneous flow conditions. The expressions used for the dispersion coefficients in the model are as follows:

$$D_{xx} = \sqrt{\frac{f}{8}\,(q_x^{\;2} + q_y^{\;2})}\;(5.9 - 5.7\,\sin^2\theta) \tag{2-36}$$

$$D_{xy} = 11.4\sqrt{\frac{f}{8}\,(q_x^{\;2} + q_y^{\;2})}\;\sin\theta\,\cos\theta \tag{2-37}$$

$$D_{yy} = \sqrt{\frac{f}{8}\,(q_x^{\;2} + q_y^{\;2})}\;(5.9 - 5.7\,\cos^2\theta) \tag{2-38}$$

where D_{xx}, D_{xy}, D_{yy} = dispersion coefficients

θ = $\tan^{-1}(q_y/q_x)$

q_x = flow in x direction

q_y = flow in y direction

The above model has been successfully tested against dye diffusion experiments in Flushing Bay, New York, and in Community Harbor, Saudi Arabia (Pagenkopf and Taylor (1985); Taylor and Pagenkopf (1981)).

A two-dimensional, finite element water quality model was developed by Chen et al. (1979), based on the earlier model by Christodoulou et al. (1976). They provided for flow-dependent anisotropic dispersion coefficients by using the following relationships:

$$D_x = \frac{\varepsilon_x^* \, q_x}{H^{1/6}} + \varepsilon_x^{**} \tag{2-39}$$

$$D_y = \frac{\varepsilon_y^* \, q_y}{H^{1/6}} + \varepsilon_y^{**} \tag{2-40}$$

where ε_x^* and ε_y^* are user-defined constants as are ε_x^{**} and ε_y^{**}, the latter being provided for additional dispersion effects such as wind and marine traffic.

Whether the two-dimensional model in question utilizes constant or flow-dependent dispersion coefficients, the dispersion mechanism is usually somewhat dependent on factors typically beyond user control, such as numerical instabilities and grid size averaging effects. It is therefore