Special Publication SJ94-SP17

St. Johns River, Florida
Water Quality Feasibility Study
Phase I Interim Report

Volume VI

Review and Evaluation of Hydrodynamic Modeling for the Lower St. Johns River Estuary

Review of Water Quality Monitoring and Recommendations for Water Quality Modeling of the Lower St. Johns River

U.S. Army Corps of Engineers
Jacksonville District
South Atlantic Division

St. Johns River Water Management District
Palatka, Florida

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Review and Evaluation of Hydrodynamic Modeling for the Lower St. Johns River Estuary

FINAL DRAFT

REVIEW AND EVALUATION OF HYDRODYNAMIC MODELING FOR THE LOWER ST. JOHNS RIVER ESTUARY

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AND THE ST. JOHNS RIVER WATER MANAGEMENT DISTRICT

September 1993

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1. INTRODUCTION

The St. Johns River Water Management District (SJRWMD) desires to quantify the hydrodynamic, sediment transport and water quality processes of the Lower St. Johns River Estuary (LSJRE). The long term management goals of the SJRWMD encompass pollution load reduction, control of eutrophication, water supply planning, and enhancing the overall health of the estuarine ecosystem. SJRWMD engineers, scientists and planners require information about the physical, chemical, and biological response of the system to changing environmental conditions, including land use modification, release of industrial and domestic effluents, channel modification, and water management operations. The SJRWMD is considering the use of numerical hydrodynamic, sediment transport, and water quality modeling tools to quantify these processes and to provide information for making long-term water management decisions.

The dominant mechanisms for distributing water borne materials in estuaries are advection by currents and turbulent mixing. An engineer must first understand the hydrodynamic processes that dominate an estuarine system before he or she can quantify the transport of particulate and dissolved materials. Over the past 25 years, numerical hydrodynamic modeling of rivers and estuaries has become accepted as a reliable engineering practice. Advances in computer technology have enabled numerical models to reproduce observed circulation patterns at spatial scales from tens of feet to thousands of feet. Efforts to model the fate of sediments, chemicals, and organisms in an estuary have followed. Transport models use velocity and water surface elevation data generated by a hydrodynamic model to advect and disperse material during simulation. Therefore, the success of a water quality or sediment modeling program ultimately depends upon the accuracy and reliability of the underlying hydrodynamic model.

A variety of modeling technologies have been developed to handle the inherent complexities of the estuarine hydrodynamic equations. Each type of model incorporates certain assumptions and simplifications of the prototype system. The science of numerical hydrodynamic modeling has advanced to the point where most of the underlying assumptions are well documented, and the conditions under which they apply are understood. Existing hydrodynamic models range from complex three-dimensional models to simple one-dimensional models. Although complex models generally incorporate fewer limiting assumptions, simpler models are easier to apply and require fewer resources. The choice of an appropriate hydrodynamic model for a particular estuarine system requires an evaluation of the existing data for the prototype estuary, a clear statement of the objectives of the modeling study, and an assessment of the resources available, which must include computer hardware, computer software, manpower, and field data.

Recognizing that the hydrodynamic component is critical for successful estuarine water quality and sediment transport modeling, the objective of this research is to provide information and recommend criteria for selecting a hydrodynamic model to achieve SJRWMD management goals. In support of this objective, this document reviews the state-of-the-art in hydrodynamic/salinity modeling of estuaries. Major hydrodynamic modeling technologies are compared and contrasted. The data requirements for application of a hydrodynamic model to the LSJRE are outlined. An approach for developing a system of models and monitoring programs for the LSJRE is recommended. Finally, a discussion of computer hardware and software issues that will affect the productivity of the modeling system is presented.

2. EQUATIONS OF ESTUARINE HYDRODYNAMICS

Estuarine circulation is governed by the equations for unsteady three-dimensional stratified flow. Existing three-dimensional numerical hydrodynamic models derive their formulations from the Reynolds form of the Navier-Stokes equations for conservation of momentum, the equation of mass continuity, the advection-diffusion equation for salinity and/or temperature transport, and the equation of state relating water density

to salinity and/or temperature (King, 1993). In this chapter, the governing equations are presented, and the common approximations for estuarine problems are described.

Three-dimensional Hydrodynamic/Salinity Equations

The three-dimensional Reynolds form of the Navier-Stokes equations are given below (Le Méhauté,1976). In the following equations, the overbar indicates time-averaged quantities. The time scale of integration for time-averaged quantities is larger than the time scale of random turbulent fluctuations in the flow field, but smaller than the time scale of the mean flow fluctuations due to boundary forcing and wave propagation. The following equations incorporate the Boussinesq assumption that the derivatives of density ($\partial\rho/\partial t$ and $\partial\rho/\partial x$ for example) are small. In three-dimensions, the equations are a statement of conservation of momentum in the x-direction,

$$\rho\left(\frac{\partial \bar{u}}{\partial t} + \bar{u}\frac{\partial \bar{u}}{\partial x} + \bar{v}\frac{\partial \bar{u}}{\partial y} + \bar{w}\frac{\partial \bar{u}}{\partial z}\right) =$$

[Local acceleration] [Convective acceleration]

$$-\rho\frac{\partial}{\partial x}(\bar{p} + \rho g z) + \mu\nabla^2\bar{u} - \rho\left(\frac{\partial \overline{u'^2}}{\partial x} + \frac{\partial \overline{u'v'}}{\partial y} + \frac{\partial \overline{u'w'}}{\partial z}\right) - \Gamma_x \ ;$$

[Pressure and gravity forces] [Viscous forces] [Turbulent fluctuation forces] [Tractive forces]

a statement of conservation of momentum in the y-direction,

$$\rho\left(\frac{\partial \bar{v}}{\partial t} + \bar{u}\frac{\partial \bar{v}}{\partial x} + \bar{v}\frac{\partial \bar{v}}{\partial y} + \bar{w}\frac{\partial \bar{v}}{\partial z}\right) =$$

$$-\rho\frac{\partial}{\partial y}(\bar{p} + \rho g z) + \mu\nabla^2\bar{v} - \rho\left(\frac{\partial \overline{u'v'}}{\partial x} + \frac{\partial \overline{v'^2}}{\partial y} + \frac{\partial \overline{v'w'}}{\partial z}\right) - \Gamma_y \ ;$$

and a statement of conservation of momentum in the z-direction,

$$\rho\left(\frac{\partial \bar{w}}{\partial t} + \bar{u}\frac{\partial \bar{w}}{\partial x} + \bar{v}\frac{\partial \bar{w}}{\partial y} + \bar{w}\frac{\partial \bar{w}}{\partial z}\right) =$$

$$-\rho\frac{\partial}{\partial z}(\bar{p} + \rho g z) + \mu\nabla^2\bar{w} - \rho\left(\frac{\partial \overline{u'w'}}{\partial x} + \frac{\partial \overline{v'w'}}{\partial y} + \frac{\partial \overline{w'^2}}{\partial z}\right) - \Gamma_z \ ,$$

where

x, y, z = right-handed Cartesian coordinate directions (L),

$\overline{u}, \overline{v}, \overline{w}$ = the time-averaged mean velocities in the x, y, and z directions (L/T),

u', v', w' = the turbulent fluctuation velocities in the x, y, and z directions (L/T),

t = time (T),

ρ = the density of water (M/L^3),

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

g = acceleration due to gravity acting in the -z direction (L/T^2),

μ = viscosity of water (M/LT), and

$\Gamma_x, \Gamma_y, \Gamma_z$ = summation of tractive and body forces (excluding gravity) per unit volume in the x, y and z directions (M/L^2T^2).

Tractive and body forces acting on estuarine bodies include wind stress, bed friction, and Coriolis force.

The continuity relationship in three dimensions can be written as follows (Le Méhauté, 1976):

$$\frac{\partial \overline{u}}{\partial x} + \frac{\partial \overline{v}}{\partial y} + \frac{\partial \overline{w}}{\partial z} = 0.$$

A general form of the advection-diffusion equation for salinity is

$$\frac{\partial s}{\partial t} + \overline{u}\frac{\partial s}{\partial x} + \overline{v}\frac{\partial s}{\partial y} + \overline{w}\frac{\partial s}{\partial z} - \frac{\partial}{\partial x}\left(D_x \frac{\partial s}{\partial x}\right) - \frac{\partial}{\partial y}\left(D_y \frac{\partial s}{\partial y}\right) - \frac{\partial}{\partial z}\left(D_z \frac{\partial s}{\partial z}\right) \pm \theta_s = 0,$$

where

s = salinity concentration (M/L^3),

D_x, D_y, D_z = turbulent diffusion coefficients for salinity in the x, y, and z directions (L^2/T), and

θ_s = source (+) or sink (-) for salinity (M/L^3T).

A similar equation can be written for the advection-diffusion of temperature.

An equation of state is needed to complete the system of equations:

$$\rho = F(s, T)$$

where

T = temperature, and

F(s,T) = an empirically derived relationship describing the variation of water density with salinity and temperature.

Given this system of equations, the independent variables are (x, y, z, t). The dependent variables to be solved are $(\overline{u}, \overline{v}, \overline{w}, \overline{p}, s, T)$. The time scales of estuarine modeling studies are such that it is not necessary to solve for the instantaneous turbulent fluctuation velocities, (u',v',w'). The turbulent fluctuation terms are normally parameterized so that the net effects of (u',v',w') on $(\overline{u}, \overline{v}, \overline{w}, \overline{p}, s, T)$ are described, although (u',v',w') remain unknown. Since the variables of interest are the time-averaged velocities and the time-averaged pressure, one can henceforth drop the bar notation without loss of clarity:

$$(\overline{u}, \overline{v}, \overline{w}, \overline{p}, s, T) = (u, v, w, p, s, T).$$

Typical parameterizations of the turbulent fluctuation terms are described later in this chapter.

To solve this system of partial differential equations for (u, v, w, p, s, T), a solution domain must be defined and appropriate boundary conditions applied. The solution domain for an estuarine model is

typically the wetted area of the estuary. The boundaries are positioned along the estuary shorelines and at channel cross-sections where the time series of total discharge or water surface elevation is known from gauged data. Uncertainty in the boundary condition data is common. Therefore, open boundaries should be positioned far from the targeted study area. Close-in boundary conditions cause the solution to be unduly influenced by errors in the boundary condition data. The type and extent of boundary condition data required for modeling of LSJRE flows are discussed elsewhere in this report.

Hydrostatic Pressure Assumption (Shallow Water Approximation)

Estuarine systems are considered shallow water systems because the depth of flow is much smaller than the length of the tidal wave. The flow is assumed to be nearly horizontal, and the effects of vertical momentum transport can be neglected (Luettich, et al., 1991). In other words, the time and space derivatives of the vertical velocity are small when compared to the horizontal velocity gradients. Under the shallow water approximation, the equation for conservation of momentum in the z-direction (vertical direction) reduces to the following:

$$\frac{\partial p}{\partial z} = -\rho g .$$

Thus, the pressure distribution in the vertical direction is hydrostatic.

Viscous Forces

The Reynolds equations for conservation of linear momentum includes a viscous force term, which appears as

$$\mu \nabla^2 u$$

in the x-momentum equation. A similar term is found in the y-momentum equation. This term accounts for energy transfer due to fluid molecular interactions. The order of magnitude of such energy transfers is small when compared to the turbulent energy transfers described by the turbulent fluctuation terms. In most hydrodynamic model formulations,

the viscous force term is either lumped with the turbulent fluctuation terms, or neglected. Thus the approximation

$$\mu \nabla^2 u \approx 0 \quad \text{and} \quad \mu \nabla^2 v \approx 0$$

is applied.

Reynolds Stresses

The turbulent fluctuation term of the x-momentum equation was given as

$$\rho\left(\frac{\partial \overline{u'^2}}{\partial x} + \frac{\partial \overline{u'v'}}{\partial y} + \frac{\partial \overline{u'w'}}{\partial z} \right),$$

and in the y-momentum equation

$$\rho\left(+ \frac{\partial \overline{u'v'}}{\partial x} + \frac{\partial \overline{v'^2}}{\partial y} + \frac{\partial \overline{v'w'}}{\partial z} \right).$$

The product of the fluctuation velocities is a measure of the correlation between turbulence events in each Cartesian coordinate direction. These correlations manifest themselves as directional stress components acting on the differential fluid volume, known as the Reynolds stresses (Le Méhauté,1976):

$$\rho\left(\frac{\partial \overline{u'^2}}{\partial x} + \frac{\partial \overline{u'v'}}{\partial y} + \frac{\partial \overline{u'w'}}{\partial z} \right) = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}$$

and

$$\rho\left(\frac{\partial \overline{u'v'}}{\partial x} + \frac{\partial \overline{v'^2}}{\partial y} + + \frac{\partial \overline{v'w'}}{\partial z} \right) = \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z}$$

where

τ_{ij} = the Reynolds stress component on the i plane in the j direction, for i = 1, 2, 3 and j = 1, 2 corresponding to the x, y, and z directions (M/LT^2).

The Reynolds equations for three-dimensional conservation of momentum with hydrostatic approximation, molecular viscosity neglected, and turbulent fluctuation forces expressed as Reynolds stresses, reduce to the simplified x-momentum equation,

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z}\right) = -\rho\frac{\partial}{\partial x}(p + \rho g z) - \frac{\partial \tau_{xx}}{\partial x} - \frac{\partial \tau_{yx}}{\partial y} - \frac{\partial \tau_{zx}}{\partial z} - \Gamma_x \ ,$$

the simplified y-momentum equation,

$$\rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z}\right) = -\rho\frac{\partial}{\partial y}(p + \rho g z) - \frac{\partial \tau_{xy}}{\partial x} - \frac{\partial \tau_{yy}}{\partial y} - \frac{\partial \tau_{zy}}{\partial z} - \Gamma_y \ ,$$

and statement of the hydrostatic pressure assumption ,

$$\frac{\partial p}{\partial z} = -\rho g \ .$$

Parameterizations of the Turbulent Fluctuation Terms

The Reynolds stresses can be related to the time-averaged velocity components via a turbulence sub-model. Parameterizations of the fluctuation term vary widely among estuarine hydrodynamic models. A complete discussion of turbulent stress models is beyond the scope of this report. The reader is referred to the ASCE Task Committee on Turbulence models in Hydraulic Computations (1988) for more information.

The directional components of Reynolds stress represent the correlations between the random turbulent velocity components which are a measure of the turbulent kinetic energy. These correlations, or moments, can be described by transport equations for the Reynolds stress tensor. Unfortunately, this new equation contains additional unknown moments, namely the triple correlations of turbulent velocity components and turbulent velocity-pressure correlations. Higher order systems of equations continue to generate new unknown correlations. In fact, the system of moment equations forms a hierarchy of coupled, non-linear partial differential equations that is countably infinite. Turbulence closure models use empirical information to truncate the system at the

level of first or second order moments. Three of the most commonly applied turbulence closure models are described below.

Boussinesq Eddy Viscosity Approximation

A frequently applied approximation is derived from the assumption that the Reynolds stress varies linearly with the gradient of the time-averaged velocities (Bird, et al., 1960). Under this theory, the stresses caused by random turbulent motions are analogous to Newton's law of viscosity for viscous stresses arising from molecular motions. This approximation gives rise to following:

$$\tau_{xx} = -\varepsilon_{xx} \frac{\partial u}{\partial x},$$

$$\tau_{yx} = -\varepsilon_{yx} \frac{\partial u}{\partial y},$$

$$\tau_{zx} = -\varepsilon_{zx} \frac{\partial u}{\partial z},$$

$$\tau_{yy} = -\varepsilon_{yy} \frac{\partial v}{\partial y},$$

$$\tau_{xy} = -\varepsilon_{xy} \frac{\partial v}{\partial x}, \text{ and}$$

$$\tau_{zy} = -\varepsilon_{zy} \frac{\partial v}{\partial z}$$

where

ε_{ij} = turbulent coefficient of viscosity in the i plane in the j direction, also called "eddy viscosity" (M/LT).

Unlike the molecular viscosity, the eddy viscosity is a property of the flow, and not of the fluid. The value of ε_{ij} in an unsteady flow field is therefore dependent upon time and position.

Under the eddy viscosity approximation, the turbulent fluctuation terms of the Reynolds equations become

$$-\frac{\partial \tau_{xx}}{\partial x} - \frac{\partial \tau_{yx}}{\partial y} - \frac{\partial \tau_{zx}}{\partial z} = \frac{\partial}{\partial x}\left(\varepsilon_{xx} \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_{yx} \frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_{zx} \frac{\partial u}{\partial z}\right)$$

and

$$-\frac{\partial \tau_{xy}}{\partial x} - \frac{\partial \tau_{yy}}{\partial y} - \frac{\partial \tau_{zy}}{\partial z} = \frac{\partial}{\partial x}\left(\varepsilon_{xy}\frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_{yy}\frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_{zy}\frac{\partial v}{\partial z}\right).$$

The values of the eddy viscosity components may be user specified or, as in some estuarine hydrodynamic models, may be internally computed based on semi-empirical relationships. Eddy viscosity models are well suited to describe horizontal turbulent momentum transfers in estuarine flow models.

Second Order Turbulence Closure Models

Blumberg and Oey (1985) state that the vertical Reynolds stresses (τ_{zx} and τ_{zy}) cannot be properly modeled with an eddy viscosity approach, except where data are specifically collected for adjustment of the vertical mixing coefficients. An alternative to the eddy viscosity approach is a second-moment closure model of small-scale turbulence which solves for the production, transport, and dissipation of turbulent kinetic energy. A well known example is the k-ε model (Rodi, 1987). The k-ε model contains coefficients that are taken to be constant over a given class of flows.

Another well known closure model solves equations for 1) the turbulent kinetic energy, and 2) a turbulence macro scale (Mellor and Yamada, 1982). Blumberg and Oey (1985), Johnson, et al. (1991) and others report excellent results from this turbulence closure scheme. A modification of the Mellor-Yamada scheme is frequently applied which damps mixing in highly stratified flows based using a Richardson number criterion.

Two-dimensional, Vertically Averaged Equations

A two-dimensional, vertically averaged approximation of estuarine hydrodynamics is frequently applied when the vertical velocities are negligible ($w(x,y,z) \approx 0$) and the vertical density gradients are negligible ($\rho(x,y,z,t) = \rho(x,y,t)$). This approximation introduces a major simplification to the equations, the parameterization of bottom

stress (Blumberg and Oey, 1985). The bottom stress is one of the tractive forces acting on the fluid body, and is normally parameterized using a Chezy or Mannings friction formulation.

The vertically integrated equation for continuity of mass can be written as follows:

$$\frac{\partial \zeta}{\partial t} + H\left(\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y}\right) + U\frac{\partial H}{dx} + V\frac{\partial H}{\partial y} = 0$$

The vertically averaged Reynolds equations for conservation of momentum in the horizontal directions are

$$\frac{\partial U}{\partial t} + \left(U\frac{\partial U}{\partial x} + V\frac{\partial U}{\partial y}\right) =$$

[Local acceleration] [Convective acceleration]

$$-g\frac{\partial \zeta}{dx} + \frac{1}{H\rho_o}\left[\frac{\partial}{\partial x}\int_{-h}^{\zeta}\tau_{xx}dz + \frac{\partial}{\partial y}\int_{-h}^{\zeta}\tau_{yx}dz\right]$$

[Free surface force] [Turbulent diffusion force]

$$-\left[\frac{g(\rho-\rho_o)}{\rho_o}\frac{\partial \zeta}{\partial x} + \frac{gH}{\rho_o}\frac{\partial \rho}{\partial x}\right] - \frac{1}{H}\int_{-h}^{\zeta}\Gamma_x dz$$

[Baroclinic force] [Tractive forces]

$$\frac{\partial V}{\partial t} + \left(U\frac{\partial V}{\partial x} + V\frac{\partial V}{\partial y}\right) =$$

$$-g\frac{\partial \zeta}{dy} + \frac{1}{H\rho_o}\left[\frac{\partial}{\partial x}\int_{-h}^{\zeta}\tau_{xy}dz + \frac{\partial}{\partial y}\int_{-h}^{\zeta}\tau_{yy}dz\right]$$

$$-\left[\frac{g(\rho-\rho_o)}{\rho_o}\frac{\partial \zeta}{\partial y} + \frac{gH}{\rho_o}\frac{\partial \rho}{\partial y}\right] - \frac{1}{H}\int_{-h}^{\zeta}\Gamma_y dz$$

where

ζ = free surface elevation relative to fixed datum (usually mean sea level) (L),

h = bathymetric depth relative to datum (L),

H = total water depth, $H=h+\zeta$,

U = depth averaged horizontal velocity in the x-direction, $U = \frac{1}{H}\int_{-h}^{\zeta} u dz$,

V = depth averaged horizontal velocity in the y-direction, $V = \frac{1}{H}\int_{-h}^{\zeta} v dz$, and

ρ_o = reference density of water (M/L^3).

Note that density differences are ignored unless they are multiplied by gravity. This approximation was first introduced by Boussinesq.

These equations are frequently used in an alternative form, known as the conservative form. The conservative form of the vertically averaged Reynolds equations is obtained by substituting the mass continuity equation into the Reynolds equations. Some authors report increased numerical stability when the conservative form is used, although a rigorous analysis has not been performed (Luettich, et al., 1991).

The conservative form of the vertically averaged Reynolds equations for conservation of momentum are written

$$\frac{\partial UH}{\partial t} + \frac{\partial U^2 H}{\partial x} + \frac{\partial UVH}{\partial y} =$$

$$-Hg\frac{\partial \zeta}{dx} + \frac{1}{\rho_o}\left[\frac{\partial}{\partial x}\int_{-h}^{\zeta}\tau_{xx}dz + \frac{\partial}{\partial y}\int_{-h}^{\zeta}\tau_{yx}dz\right]$$

$$-\left[\frac{Hg(\rho-\rho_o)}{\rho_o}\frac{\partial \zeta}{\partial x} + \frac{gH^2}{\rho_o}\frac{\partial \rho}{\partial x}\right] - \int_{-h}^{\zeta}\Gamma_x dz$$

and

$$\frac{\partial VH}{\partial t} + \frac{\partial UVH}{\partial x} + \frac{\partial V^2 H}{\partial y} =$$

$$-Hg\frac{\partial \zeta}{dy} + \frac{1}{\rho_o}\left[\frac{\partial}{\partial x}\int_{-h}^{\zeta}\tau_{xy}dz + \frac{\partial}{\partial y}\int_{-h}^{\zeta}\tau_{yy}dz\right]$$

$$-\left[\frac{Hg(\rho-\rho_o)}{\rho_o}\frac{\partial \zeta}{\partial y} + \frac{gH^2}{\rho_o}\frac{\partial \rho}{\partial y}\right] - \int_{-h}^{\zeta}\Gamma_y dz \ .$$

The vertically averaged advection-diffusion equation is

$$\frac{\partial S}{\partial t} + U\frac{\partial S}{\partial x} + V\frac{\partial S}{\partial y} - \frac{\partial}{\partial x}\left(\bar{D}_x\frac{\partial S}{\partial x}\right) - \frac{\partial}{\partial y}\left(\bar{D}_y\frac{\partial S}{\partial y}\right) \pm \frac{1}{H}\int_{-h}^{\zeta}\theta_s dz = 0$$

where

S = vertically averaged salinity concentration (M/L^3), $S = \frac{1}{H}\int_{-h}^{\zeta} s\, dz$, and

$\bar{D}_x, \bar{D}_y$ = turbulent diffusion coefficients for vertically averaged salinity concentration in the x and y directions (L^2/T).

Mode Splitting

The vertically averaged equations are also used to speed up the computations of some three dimensional estuarine models by a technique called "mode splitting". Mode splitting entails solving the two-dimensional vertically averaged equations for ζ, U, and V at each time step, then using the computed values to drive the equations for three dimensional momentum and salinity transport. The vertically averaged solution is referred to as the "external mode" solution, and the solution of the 3-D equations is referred to as the "internal mode" solution. This strategy is applied by Luettich, et al. (1991), Blumberg and Mellor (1987), Sheng (1986), and Johnson, et al. (1991).

Wave Continuity Equation for Vertically Averaged Flow

The primitive vertically averaged equation for conservation of mass is sometimes replaced with a wave-continuity equation (WCE). A WCE is obtained by algebraic manipulation of the primitive equations. The vertically averaged continuity equation is first differentiated with respect to time, then the spatial derivative of the conservative form of the x- and y- momentum equations are invoked to replace time derivatives of velocity that result from the differentiation. The result of this manipulation is that the continuity equation has the form of a wave equation, which may be numerically advantageous. The new equation replaces the primitive continuity equation and is solved along with the primitive momentum and the advection-diffusion equations.

Authors who use the WCE report a reduction of the $2\Delta x$ oscillations in their numerical solution (Lee and Froehlich, 1986). A $2\Delta x$ oscillation refers to numerical noise generated when a continuous solution is represented on a discrete solution domain. The $2\Delta x$ wavelength is the smallest wavelength that can be resolved by the discretization. Freeman (1992) indicates that the reduction of $2\Delta x$ oscillations may occur at the expense of solution accuracy, particularly for riverine flow problems.

Most authors using the wave-continuity equation neglect horizontal momentum diffusion terms. The additional differentiation required to obtain the WCE produces third order terms which complicate the model solution. The elimination of these terms does not have serious consequences in the solution of certain open water problems that are dominated by advection and tidal forcing, such as coastal flows and flows in large embayments. However, flows with complex land boundaries and bathymetry, such as rivers, harbors, marinas, bridge piers, and islands are shear dominated and the horizontal momentum terms cannot be neglected.

This form of the equation also affects the way boundary conditions are specified. Wave continuity equations normally use water surface elevation boundary conditions and/or wave absorption/reflection boundary

conditions at all open boundaries, rather than specifying total discharge at open river boundaries. Estuaries that transition to riverine flow along the length of the channel experience a mix of tidal forcing and gravity wave propagation due to freshwater inflow. The wave equation formulation is not well suited to landward boundary conditions of this type.

Constant Density, Vertically Averaged Approximation

Certain coastal embayments do not have significant lateral density gradients because freshwater inflow is small compared to sea water contributions, and temperature is essentially constant. In such cases, a vertically averaged, constant density approximation is frequently applied, i.e. $\rho(x,y,t) = \rho_o$. This approximation eliminates the need to solve for the transport of salt and temperature. The equations resulting from this approximation are the vertically integrated continuity equation (also called the free surface equation),

$$\frac{\partial \zeta}{\partial t} + H\left(\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y}\right) + U\frac{\partial H}{dx} + V\frac{\partial H}{\partial y} = 0;$$

the x-momentum equation,

$$\frac{\partial U}{\partial t} + \left(U\frac{\partial U}{\partial x} + V\frac{\partial U}{\partial y}\right) = -g\frac{\partial \zeta}{dx} + \frac{1}{H\rho_o}\left[\frac{\partial}{\partial x}\int_{-h}^{\zeta}\tau_{xx}dz + \frac{\partial}{\partial y}\int_{-h}^{\zeta}\tau_{yx}dz\right] - \frac{1}{H}\int_{-h}^{\zeta}\Gamma_x dz;$$

and the y-momentum equation,

$$\frac{\partial V}{\partial t} + \left(U\frac{\partial V}{\partial x} + V\frac{\partial V}{\partial y}\right) = -g\frac{\partial \zeta}{dy} + \frac{1}{H\rho_o}\left[\frac{\partial}{\partial x}\int_{-h}^{\zeta}\tau_{xy}dz + \frac{\partial}{\partial y}\int_{-h}^{\zeta}\tau_{yy}dz\right] - \frac{1}{H}\int_{-h}^{\zeta}\Gamma_y dz.$$

Two-dimensional Laterally Averaged Equations

The flow characteristics of estuaries that are narrow and non-branching may be sufficiently uniform in the cross-channel direction to permit laterally averaging. Lateral averaging preserves the terms that

describe vertical density structure and baroclinic forcing, so that this approximation applies when vertical stratification dominates the system.

The laterally averaged equations in conservative form are the continuity equation (Ford, Wang and Cheng, 1990),

$$\frac{\partial(Bu)}{\partial x} + \frac{\partial(Bw)}{\partial z} = 0$$

where B(x,z) is the width of the estuary;

the longitudinal momentum equation,

$$\frac{\partial(Bu)}{\partial t} + \frac{\partial\left(Bu^2\right)}{\partial x} + \frac{\partial(Bwu)}{\partial z} = -gB\frac{\partial\zeta}{\partial x} - \frac{gB}{\rho_o}\int_z^{\zeta}\frac{\partial\rho}{\partial x}dz' + \frac{1}{\rho_o}\left(\frac{\partial\tau_{xx}}{\partial x} + \frac{\partial\tau_{zx}}{\partial z}\right) - \frac{\Gamma_x}{\rho_o}$$

where here Γ_x includes side friction, bottom friction and longitudinal wind stress, but does not include Coriolis effects;

the vertically integrated continuity equation,

$$B_{@z=\zeta}\frac{\partial\zeta}{\partial t} + \frac{\partial}{\partial x}\int_{-h}^{\zeta}(Bu)dz = 0;$$

the advection-diffusion equation for salinity (or similarly for temperature),

$$\frac{\partial(Bs)}{\partial t} + \frac{\partial(Bus)}{\partial x} + \frac{\partial(Bws)}{\partial z} = \frac{\partial}{\partial x}\left(BD_x\frac{\partial s}{\partial x}\right) + \frac{\partial}{\partial z}\left(BD_z\frac{\partial s}{\partial z}\right) \pm \theta_s;$$

and an equation of state,

$$\rho = F(s,T).$$

One-dimensional Equations

Estuaries that are narrow, non-stratified, and non-branching may be modeled by the one-dimensional equations for unsteady, open channel flow. Estuaries that are narrow, non-stratified and branching may be modeled by a one-dimensional channel network. The equations for these models are obtained by integrating the three-dimensional equations in the lateral (y) and vertical

(z) directions. For branched models the channel junctions are subjected to an additional constraint. Usually the water surface elevation is constrained to be equal for all channels at the junction, although an equal energy constraint can also be used.

The one-dimensional equations of estuarine hydrodynamics are the continuity equation

$$\frac{\partial \zeta}{\partial t} + H \frac{\partial \overline{U}}{\partial x} + \overline{U} \frac{\partial H}{\partial x} = 0$$

where

$\overline{U}$ = the cross-section averaged velocity;

the one-dimensional Reynolds equations for conservation of momentum in the longitudinal direction

$$\frac{\partial \overline{U}}{\partial t} + \overline{U} \frac{\partial \overline{U}}{\partial x} = -g \frac{\partial \zeta}{dx} + \frac{1}{H\rho_o} \left[\frac{\partial \overline{\tau}_{xx}}{\partial x} \right] - \left[\frac{g(\rho - \rho_o)}{\rho_o} \frac{\partial \zeta}{\partial x} + \frac{gH}{\rho_o} \frac{\partial \rho}{\partial x} \right] - \frac{1}{H} \overline{\Gamma_x}$$

where

$\overline{\tau}_{xx}$ = the cross-section averaged Reynolds stress in the longitudinal direction, and

$\overline{\Gamma_x}$ = the longitudinal tractive forces;

the one-dimensional advection-diffusion equation for salinity

$$\frac{\partial \overline{S}}{\partial t} + \overline{U} \frac{\partial \overline{S}}{\partial x} - \frac{\partial}{\partial x} \left(\overline{\overline{D_x}} \frac{\partial \overline{S}}{\partial x} \right) \pm \overline{\theta_s} = 0$$

where

$\overline{S}$ = the cross-section averaged salinity,

$\overline{\overline{D_x}}$ = the one-dimensional diffusion coefficient for salinity, and

$\overline{\theta_s}$ = the cross-section sources and sinks for salinity;

and an equation of state

$$\rho = F(\bar{S}, \bar{T}).$$

Multi-dimensional Approximations

Certain models are capable of applying combinations of 1-D, 2-D vertically averaged, 2-D laterally averaged, and 3-D approximations in the same computational mesh. Transitions between the various approximations are handled by special rules, which act as internal constraints on the governing equations. A multi-dimensional approach is advantageous when the estuary encompasses a large, diverse area.

The major advantage of multi-dimensional grids is computational cost. The user is permitted to use a three-dimensional approximation in key regions that are characterized by vertical stratification, wind driven circulation, and secondary currents. The user can apply a vertically averaged approximation in regions that are shallow and vertically well mixed. As stated in the section on governing equations, moving the boundary conditions away from the area of interest is desirable to improve solution accuracy. Multi-dimensional models permit specification of boundary conditions far upstream in the landward direction, and far into the open ocean without a large increase in the number of computational nodes. Some examples of multi-dimensional models follow:

Model / Authors	Multi-dimensional Capabilities	References
RMA-10 / King	3-D 2-D vertically averaged 2-D laterally averaged 1-D	King, 1993
CH3D-WES / Sheng and Johnson	3-D 2-D laterally averaged	Sheng, 1993 Johnson, et al., 1991
TRIM3D / Cheng and Casulli	3-D 2-D vertically averaged	Casulli and Cheng, 1992

Spectral Methods

Periodic, tidal forcing dominates estuarine circulation and may be approximated by harmonic solutions of the equations of estuarine hydrodynamics. A frequency domain solution propagates the water surface elevation and the velocities in time by means of harmonic series. The principal benefit of this approach is efficiency for long-term simulations (Walters, 1987).

The harmonic amplitudes and frequencies of boundary condition data needed for a spectral model can be generated from analysis of field data. Time histories are subjected to harmonic analysis using a least squares procedure. Alternatively, the amplitudes and frequencies of the astronomical tide constituents can be used when tidal forcing is known to dominate the flow field. Spectral models are particularly useful for predicting regional tide levels. Spectral models are not recommended for examining alternative channel geometries, infrequent storm events, or extreme tide events because the harmonic constants are based on the historical record and therefore cannot express the physics of hypothetical events or altered geometry.

3. NUMERICAL SOLUTION TECHNIQUES

In this chapter, common numerical solution techniques for the solution of estuarine hydrodynamic equations are briefly described.

Discretization of the Solution Domain

The governing equations described in Chapter 2 do not lend themselves to analytic solutions. Furthermore, the flow domains that are of interest, i.e. the estuaries, rivers and embayments, are geometrically complex. Therefore, the continuous physical flow domain is mapped onto a discrete, finite computational grid or mesh on which approximate numerical methods can be applied. The mesh is intended to capture significant geometric and bathymetric features of the estuary.

Computational grids for solving flow problems are typically fixed domain grids. That is, the reference points for solution, called nodes

or cells, have fixed Cartesian coordinates (x, y, z). The shallow water equations introduce a complication to this approach because the free surface elevation is unknown prior to solution. Therefore, most three-dimensional solutions of the shallow water equations have fixed nodes in the horizontal directions (x, y) and moving nodes in the vertical direction (z) (although there are some exceptions). Two-dimensional laterally averaged models use fixed-coordinate longitudinal nodes (x-direction) and moving vertical nodes (z-direction). Two-dimensional vertically averaged models and one-dimensional models generally employ grids that are fixed in space (x and y directions). Along with spatial coordinates, physical characteristics of the estuary such as bed roughness, tributary inflow, and wind forcing can be assigned by node.

Computational grids are characterized as being either "structured" or "unstructured" (Fletcher, 1987). Structured grids have nodes which can be referenced according to a system of indices. For a three-dimensional solution, three indices are required, (i,j,k), where i and j refer to an ordering of the nodes in the horizontal plane and k refers to an ordering of the vertical nodes. The grid for a two-dimensional laterally averaged solution requires two indices per node, (i,k), and a two-dimensional, vertically averaged solution requires two horizontal indices per node, (i,j). A one-dimensional solution uses only one index per node (i). An advantage of the structured grid system is that adjacent nodes are easily referenced by incrementing the indices. In some cases, this attribute has been exploited to increase computational efficiency.

The direction of the indices in a structured grid does not necessarily coincide with the Cartesian coordinate directions, although it may. "Cartesian grids" are those structured grids that have indices which coincide with the coordinate directions. "Curvilinear grids" are those structured grids which have indices that follow another, user defined set of index directions. Curvilinear coordinate systems require that the governing equations be transformed to a new, local coordinate system. In general, such transformations generate extra terms containing cross-transform derivatives. The higher order cross-

transformation terms are usually neglected, so that some error is incurred when coordinate transforms are introduced.

The term "boundary fitted" is used to describe structured grids that are curved to fit the domain boundaries. Cartesian grids are not boundary fitted. Instead, nodes that lie outside the boundary are simply omitted, leaving a jagged or "stepped" edge along the estuary shorelines.

Unstructured grids have nodes which cannot be referenced by index. Nodes are placed anywhere in the domain that enhances the system map. A system to keep track of node numbers and node connections is adopted to store nodal information and to identify neighboring nodes. Thus an additional bookkeeping effort is required when unstructured grids are used, but the modeler is permitted more flexibility for mapping the computational domain than can be achieved with a structured grid system. Unstructured grids are advantageous for describing complex geometries and for adding local grid detail.

Unstructured grids are organized into "elements" or "volumes" by connecting the nodes. One dimensional unstructured grids have lines connecting the nodes. The element shapes for a two-dimensional solution are normally limited to triangles and quadrilaterals, although other polygon shapes are theoretically possible. When the solution is extended to three dimensions, the resulting volumes may include tetrahedra, pyramids, wedges, and parallelepipeds. The allowable element shapes for any particular estuarine hydrodynamic model are defined by the author of the code. Some codes allow for a variety of polygon shapes, while others limit the user to only one type of element.

Numerical Methods

The equations of estuarine hydrodynamics are solved by one of three numerical solution techniques: 1. finite difference methods; 2. finite element methods; and 3. finite volume methods. Many variants of each approach exist. The details of each implementation will affect solution efficiency, accuracy, and ease of use. Each solution method

has its proponents and its detractors, but accurate and efficient solutions of the shallow water equations have been developed using all three of these methods.

To the end user of an estuarine hydrodynamic model, the method of solution is most apparent during grid development. Finite difference solutions use structured grids exclusively. Both finite element methods and finite volume methods may use either structured or unstructured grids, but normally employ unstructured grids to exploit their flexible mapping capabilities.

Grid Resolution

Grid resolution refers to the spacing of the computational nodes. The objectives of the modeling study will determine the amount of resolution required. For example, a node spacing on the order of 1000 feet may be sufficient to study the general circulation patterns in the Lower St. Johns River. A node spacing on the order of 100 feet would be required to study the circulation in a harbor or marina. Increased grid resolution (reduced node spacing) is required to define flow around channel bends, around peninsulas and islands, and around man-made structures. Grid resolution is also dependent upon the spatial distribution of depths, sediment types, channel roughness, and water quality sources.

The numerical techniques used to solve the governing hydrodynamic equations are subject to approximation error arising from discretization of a continuous domain. The magnitude of the error increases with the distance between nodes. Small node spacings adjacent to large node spacings in the same grid are particularly disadvantageous. Numerical error is reduced when grids are graded to have small node spacings in the study focus area, then transition gradually to larger spacings away from the focus area. This technique is known as local grid refinement. Local grid refinement is easier to achieve using an unstructured grid, because the nodes numbers are not tied to an index. When adding local refinement to a structured grid, the entire grid must be reworked. Such grids are referred to as "stretched" finite difference grids. Some

structured grid models do not permit local grid refinement. Instead, the node spacing over the entire grid is reduced in order to capture local effects.

The advantages and disadvantages of each grid type are summarized below:

Grid Type	Advantages	Disadvantages
Structured Cartesian	1. Easy to set up 2. Nodes identified by index are easy to locate 3. Amenable to fast, efficient solution algorithms 4. No coordinate transformations required	1. Jagged land/water boundaries 2. Grid stretching required for local refinement 3. May not represent complex geometries accurately 4. Node placement is fixed by spacing
Structured, curvi-linear, boundary fitted	1. Nodes identified by index are easy to locate 2. Land/water boundar-ies are represented accurately	1. Difficult to set up 2. Grid stretching required for local refinement 3. Coordinate trans-formations required 4. Some limitations on node placement
Unstructured	1. Node placement may be chosen to maximize map detail 2. Land/water boundar-ies are represented accurately 3. Easy to achieve local refinement	1. Difficult to set up 2. Nodes identified by number can be hard to locate 3. Historically these methods are less computationally efficient.

Time Stepping Schemes

The governing equations of estuarine hydrodynamics are discretized in time, as well as in space, to be solved numerically. Although space discretization lends itself to different solution techniques (finite difference, finite element, or finite volume), time derivatives are almost always represented by a finite difference approximation. Several different temporal finite difference schemes are being used in estuarine modeling. The choice of a temporal difference relation has consequences in terms of the order of numerical error in the model, the size of the time step permitted, and the type of matrix solver required.

Current estuarine hydrodynamic models may use an explicit finite difference formulation, an implicit finite difference formulation, or a semi-implicit finite difference formulation. Explicit methods rely on information from the previous time step to solve the system of simultaneous equations at the current time step. The problem is thus reduced to a series of algebraic equations with one unknown per equation. Implicit methods endeavor to solve the full system of equations simultaneously at the current time step. For a system of non-linear equations such as the shallow water equations, an implicit method must use an iterative solution technique, such as the Newton-Raphson method. Semi-implicit methods are hybrid methods that take some information from the previous time step, and some from the current time step. The advantage of semi-implicit methods is that they can be devised to reduce the system of simultaneous non-linear equations to a system of simultaneous linear equations. Many algorithms have been developed to quickly solve systems of linear equations.

Explicit and semi-implicit formulations for the non-linear shallow water equations include stability criterion that limit the permissible length of time step for simulation. The time step for an implicit formulation is not limited by stability constraints. Consequently, an explicit formulation requires more time steps per tidal simulation than an implicit scheme.

For most explicit schemes, the time step is constrained by the time required for a gravity wave to travel between adjacent nodes. Therefore, the maximum permissible time step for simulation is limited by the minimum node spacing, denoted Δx_{min} , as follows:

$$\Delta t \leq \frac{\Delta x_{min}}{c}$$

where c is the celerity of a gravity wave given by

$$c = \sqrt{u^2 + v^2} \pm \sqrt{gH} .$$

This time step restriction is known as the Courant-Friedrichs-Lewy condition. Time steps reported in the literature for explicit formulations of the estuarine hydrodynamic equations vary from 15 seconds to 2 minutes.

Semi-implicit schemes are also subject to stability restrictions. Semi-implicit schemes typically linearize the system of equations by evaluating some terms at time "t" and other terms at time "t+Δt". Weighted averaging between time steps can also be used to develop a semi-implicit scheme. The stability criteria for a semi-implicit formulation depend uniquely upon the terms that are linearized and/or the method of weighting values between time steps. Time steps reported in the literature for semi-implicit formulations range from 30 seconds to 15 minutes.

Although implicit schemes are not constrained by stability criteria, the time step must be short enough to resolve important features of the tidal signal at estuary boundaries. For example, a simple 12 hour tide may be described by hourly point values of water surface elevation at the ocean boundary. A 15 minute time step may be necessary to resolve shoreline movement if the estuary has significant expanses of tidal flats subject to wetting and drying over the tidal cycle.

Computational Efficiency

Computational effort required for a numerical solution algorithm is related to the number of mesh nodes, the number of time steps and the number of operations required per time step. Explicit schemes have the advantage of reducing a system of non-linear partial differential equations to a series of algebraic evaluations, which are fast to compute. More computational effort is required to perform the matrix inversion to solve a linear system of equations which results from certain semi-implicit formulations of the shallow water equations. Implicit schemes are the most computationally intensive because the fully non-linear system of equations is solved at each time step, requiring non-linear iteration as well as matrix inversion within iterations.

Unfortunately, a simple formula for determining computational efficiency is not possible. The time required to solve a particular estuarine flow problem is a function of the following factors: number and spacing of computational nodes, number of time steps required, linearized or fully non-linear form of the governing equations, time stepping scheme, structured or unstructured grid, and matrix solution routine. The efficiency of a solution is also largely application dependent. Physical characteristics of an estuary will dictate the degree of sophistication required to achieve a satisfactory simulation. Actual central processor unit (cpu) time must be determined on a case by case basis because of the wide variety of time stepping schemes and matrix solution algorithms currently available.

4. CURRENT ISSUES IN HYDRODYNAMIC MODELING

Westerink and Gray (1991) have presented a review of recent progress in surface water modeling. The authors identify several issues that are currently under investigation within the modeling community. These issues include resolution of sharp fronts, supercritical flows, wetting and drying of land boundaries, and treatment of the convective terms. Other issues of current interest include the lateral momentum

transport terms, vertical coordinate transformations, residual flows, and model verification and testing.

Lateral Momentum Transport

Representation of the lateral stresses (horizontal turbulent fluctuation terms) is necessary to induce horizontal circulation in steady flow simulations (Lee and Froehlich, 1986). In estuarine flows, these terms are an order of magnitude smaller than the vertical turbulent diffusion terms (Casulli and Cheng, 1992). Eddy viscosity formulations have been found to adequately represent the lateral Reynolds stresses at commonly used grid resolutions.

Wave equation formulations of the two-dimensional, vertically averaged shallow water equations generally omit lateral momentum transport entirely. This is justified only for unsteady flow in very shallow water bodies having large horizontal dimensions and smooth bathymetry such as lakes, large embayments, and inland seas (Lee and Froehlich, 1986). Freeman (1992) found that the wave equation model was unstable for riverine systems because lateral momentum transport is neglected.

Large values of lateral eddy viscosity have been used to suppress model instabilities (Lee and Froehlich, 1986). This technique is not recommended because real circulation induced by the convective velocities will also be suppressed. Experience dictates that a grid which is sufficiently resolved is insensitive to the magnitude of the eddy viscosity coefficients (within a realistic range). Model sensitivity analyses should be used to determine the overall effect of the eddy viscosity terms, and to distinguish the lateral momentum transport from numerical diffusion in the solution.

Wetting and Drying

The fluctuating water surface elevation that characterizes estuarine flows can produce intermittent inundation of gently sloping shorelines, tidal marshes and tidal flats. The variable extent of the flow domain is not accurately represented in all estuarine flow models.

Certain models require that the computational domain remain wet throughout simulation. Of the models that do represent flooding and drying, several successful techniques for computing the moving shoreline have been developed.

Proper simulation of intermittently flooded domains can have a significant impact on the computed tidal prism and the characteristic shape of the tidal signal. The capability to simulate intermittent flooding is required for estuaries with significant wetting and drying of the shoreline boundaries. Intermittent flow models are being used extensively for the design of wetland restoration projects.

Vertical Coordinate Transformations

Because the water surface elevation is unknown *a priori*, three-dimensional hydrodynamic models and two-dimensional laterally averaged models use a vertical coordinate transform to preserve the fixed computational grid structure. The most commonly applied vertical coordinate transforms are the σ-transform and the z-transform.

The σ-transform fixes the number of vertical node points so that the number of vertical layers is equal throughout the grid, regardless of depth. The total depth, H, is then mapped to a grid with uniform unit depth using a local coordinate stretching algorithm. The result is a uniform grid with flat bottom and flat surface. A persistent problem has been noted for certain applications of the σ-transform. In stratified flows, spurious secondary circulations have been observed due to truncation of the second order derivatives in the transformed equations. The result of these circulations is artificial diffusion of the salinity front. These problems are particularly pronounced in estuaries that have steep bathymetry breaks, such as dredged channels that are cut through shallow bays (Johnson, et al., 1991). The σ-transform is most successful in estuaries with smoothly varying bathymetry.

The z-transform was introduced to alleviate problems encountered using the σ-transform. The z-transform retains the original bottom

profile but maps the modulation of the water surface to a constant elevation (King, 1993). This transform has the additional benefit of permitting the number of vertical layers to vary over the grid. The transformation is defined as

$$x' = x,$$

$$y' = y, \text{ and}$$

$$z' = (z + h)\frac{h}{H} .$$

Resolution of Sharp Fronts

Sharp density fronts can occur at the interface between sea water and freshwater, between sediment laden water and clear water, and between waters of different temperatures. A sharp front also characterizes the hydraulic jump which occurs between regions of supercritical and subcritical flow. Concentration fronts occur in water quality and sediment transport modeling. Numerical solution of the sharp front problem introduces discretization error which typically smears the interface between high and low concentration areas.

Techniques that have been proposed to handle sharp fronts include upwinding schemes, higher order interpolation methods in finite elements, and increased grid resolution. Upwinding is a technique by which the weight functions used to derive the numerical method are more heavily weighted toward the upstream nodes than towards the downstream nodes. Upwinding reduces numerical oscillations near the sharp front, but the accuracy of the numerical method may be impaired in the rest of the solution domain (Lee and Froehlich, 1986). Higher order interpolation correctly maintains the sharpness of the front, but increases oscillations in the vicinity of the front. New techniques are being developed to apply upwinding in the vicinity of a sharp front where the solution is not smooth, and higher order interpolation in the rest of the domain where the solution is smooth. These hybrid methods take advantage of the positive features of both techniques. To date, sharp fronts have been handled most successfully by increasing grid

resolution. Future developments may include adaptive gridding (the automatic generation of a locally refined grid) and particle tracking schemes.

Treatment of the Convective Term

The convective terms are subject to discretization error (numerical diffusion) where velocity gradients exist. Numerical dispersion is a term that is used to describe errors in the speed of wave propagation. Dissipation is used describe errors in amplitude. The combination of these effects is known as numerical diffusion.

The representation of velocity gradients over a discrete grid is similar to the sharp front problem for concentration and density gradients. Equivalent remedies have been proposed: upwinding, higher order interpolation, and increased grid resolution. Lee and Froelich (1986) point out that most investigators find that *ad hoc* corrective methods are not required when grid resolution is sufficient. Most recently, Eulerian-Lagrangian schemes have been developed to alleviate numerical diffusion problems in the convective terms.

The equations presented in Chapter 2 are derived from an Eulerian viewpoint. That is, the equations describe the movement of a fluid past an observer who is fixed in space. A second approach, the Lagrangian point of view, describes the movement of a fluid as perceived by an observer traveling with the fluid. Lagrangian approaches are advantageous because there is no numerical diffusion introduced in the convective term (Cheng, et al., 1984). However, it is impractical to compute hydrodynamic flows from a strictly Lagrangian frame of reference because the fluid mass becomes distorted as it travels through space and time.

Several authors have developed hybrid Eulerian-Lagrangian (E-L) approaches for solution of transport problems (Westerink and Gray, 1991). E-L methods use a fixed grid, as with the Eulerian formulation, but use a Lagrangian formulation to track the movement of a fluid parcel over one time step. Fluid parcels are associated with a fixed node, and

the net movement over the time step is backtracked to the nodal position. At the next time step, a new fluid parcel is associated with the node and its progress is traced. E-L methods have been used to convect momentum, and to calculate convection of water quality constituents. E-L methods introduce some artificial viscosity, but are less dissipative than fully Eulerian solutions.

Supercritical Flows

Estuarine flow models are restricted to sub-critical flow. Super-critical flow is sometimes encountered in certain high-velocity flood control channels, and flow control structures such as weirs. Several estuarine flow models include options for simulating flow control structures by means of a stage-discharge relationship or other empirical formula. Super-critical flow simulation is not discussed in this review because it is not required for estuarine flow simulation in the LSJRE.

Residual Flows

Residual flows refer to the net transport of fluid (or conservative tracer moving with the fluid) over a series of tidal cycles. The time scale of interest for water quality transport is typically on the scale of weeks or months (Cheng, 1990). Although displacements due to tidal circulation can be large, it is often found that the net displacement or long-term transport of particles is quite small. Estuarine hydrodynamic models are reliable for simulation of currents on tidal time scales, but may accumulate error due to numerical diffusion and round-off during long-term simulations.

Cheng (1990) has presented a survey of methods for determining long-term transport in estuaries. Estuarine hydrodynamic models are frequently used to compute long-term transport, with the application of time filters, drogue tracking algorithms, and direct simulation. The Lagrangian residual current is frequently used to describe the net non-tidal transport in estuarine systems. The accuracy of long-term simulations is difficult to check, but such simulations are frequently used for evaluation of alternative planning scenarios. Alternative

management plans can be compared to the base plan to determine the direction of change resulting from management procedures. Greater accuracy and reliability of long-term transport predictions is an area of active research in the estuarine modeling community.

Model Testing and Verification

Methods for model testing and verification have not been standardized. In general, comparisons of velocities and water surface elevations with field data have been used to demonstrate model accuracy. Unfortunately, field verification is not a perfect predictor of model accuracy. Models can be tuned to match certain sets of field data by adjustment of coefficients or modification of the numerical method. There may be insufficient data to independently verify the model for different field conditions. The analysis is further complicated by uncertainties in the field data. In such a case, verification must be coupled with sensitivity analyses to determine model dependence on the specified parameters. The model should be capable of reproducing known behaviors of the system, such as ebb predominance, even if knowledge of the behavior is mostly qualitative.

Field verification is nonetheless important for engineering applications, where model results are used to determine design conditions. It has been shown that tidal water surface elevations are easily reproduced. Velocity magnitudes and directions are more difficult to verify, and may require iteration between field measurements, parameter modification, and model prediction. A concurrent program of hydrodynamic simulations and field data collection can result in an improved understanding of estuarine physical processes.

5. COMPATIBILITY WITH SEDIMENT TRANSPORT AND WATER QUALITY MODELS

The velocity, salinity, temperature and water surface elevation results generated by the hydrodynamic model are used to drive the transport of sediment and water quality in subsequent modeling efforts. Phenomenologically, the physical processes of sediment and water quality transport are not decoupled from the hydrodynamic processes. Erosion

and deposition of sediment in the channel bed alter the flow characteristics, and both sediment load and water quality constituent concentration can affect water density. For modeling purposes, decoupling is often used because the time scale of interest for transport processes is generally longer than the time scale of tidal variation. In most cases, the error introduced due to decoupling is minor.

In practice, a numerical interface is used to exchange information between the hydrodynamic model and the transport models. Some authors have developed specific interfaces to link their hydrodynamic model with related transport codes. Generic interfaces have been used to link hydrodynamic models with well known water quality models such as those used by the Environmental Protection Agency. Model interfaces can be inconvenient, and may introduce additional numerical errors resulting from the interpolation and time filtering that may be imbedded in the interface.

The ability to exchange information between models is necessary to the overall success of a comprehensive estuarine modeling program. Few existing estuarine models have a fully developed interface with a sediment transport model and a water quality model. Of those that do, the associated transport models may be oversimplified or inadequate for the modeling program objectives. As part of a comprehensive modeling program, interface development and compatibility with transport models must be carefully considered.

Water quality models vary widely in capabilities. Some attributes of water quality models to be considered are listed below:

i. conservative constituent transport,

ii. first and second order reaction kinetics,

iii. nutrient cycling (Nitrogen, Phosphorous, Potassium and their various molecular forms),

iv. phytoplankton dynamics (attached species and/or floating species),

v. benthic exchange dynamics,

vi. contaminant adsorption and resuspension linked to sediment dynamics, and

vii. heat budget.

Objectives of the water quality modeling program must be clearly outlined in order to select an appropriate model. A detailed review of existing models is recommended. Similar precautions are recommended for the selection of a sediment transport code. Some characteristics of sediment models to be considered are

i. suspended sediment transport,

ii. bed load transport,

iii. cohesive and non-cohesive sediment,

iv. vertical erosion/deposition functions (bed scour and accretion),

v. bed evolution (consolidation) functions,

vi. multiple grain sizes of non-cohesive sediments, and

vii. lateral erosion/deposition (bank failure).

6. ESTUARINE HYDRODYNAMIC/SALINITY MODELS

An objective of this research is to review estuarine hydrodynamic models that may apply to the LSJRE system. With one exception, only three-dimensional models and modeling systems are considered here. All of the models reviewed in this chapter have corresponding two-dimensional vertically averaged capabilities, and some have laterally averaged and one-dimensional capabilities as well. The three-dimensional model will be the state-of-the-art hydrodynamic tool within the three to five year time frame that the LSJRE is considering for model development. Therefore, modeling systems that do not demonstrate potential for three-dimensional development within that time are not reviewed.

ESTUARINE HYDRODYNAMIC MODEL

Author(s): Alan F. Blumberg and George F. Mellor

Organization: Dynalysis of Princeton, Princeton, New Jersey

Contributors (modifications and enhancements):

Name of model: ECOM (Estuarine and Coastal Ocean Circulation Model)

Related models: ECOM, Barotropic Version (2-D vertically integrated)

Remarks:

The ECOM models are some of the earliest developed estuarine flow models, and have evolved to take advantage of new technologies. Both Cartesian and curvilinear versions are available. The ECOM models interface with water quality models developed and applied by Hydroqual, Inc.

Dimensionality: 3-D

Governing equations: Fully non-linear Reynolds form of Navier Stokes with hydrostatic approximation
Continuity of Mass
Advection-Diffusion of Salinity
Advection-Diffusion of Temperature
Equation of State

Turbulence sub-model:

Horizontal: Eddy viscosity

Vertical: Eddy viscosity calculated according to second-moment turbulence closure of Mellor and Yamada (1982)

Time-stepping scheme: Split mode solution:

1. Explicit finite difference for the external mode (vertically averaged) solution

2. Leapfrog, semi-implicit finite difference scheme for internal mode (baroclinic) solution. A weak filter is applied at each time step.

Numerical solution technique: Finite difference

Type of grid: Orthogonal, curvilinear, staggered, boundary fitted, structured

Coordinate transformations:

Vertical: σ-coordinate system

Horizontal: curvilinear, boundary fitted

Example applications: Delaware Bay; Hudson-Raritan Estuary; Gulf of Mexico

Typical Δt for 3-D baroclinic circulation:

10 sec (external mode)

10 min (internal mode)

Reference: Blumberg and Mellor, 1987

Blumberg and Oey, 1985

ESTUARINE HYDRODYNAMIC MODEL

Author(s): Ian P. King

Organization: University of California, Davis, California

Contributors (modifications and enhancements):

USACE Waterways Experiment Station (WES), Vicksburg, MS

Name of model: RMA-10 (3-D hydrodynamics and conservative constituent transport)

Related models: RMA-2 (2-D vertically averaged hydrodynamics)

RMA-4 (2-D water quality transport)

RMA-7 (2-D laterally averaged hydrodynamics)

STUDH (2-D vertically averaged sediment transport)

SED-8 (multi-dimensional sediment transport)

Remarks:

This is the only commercially available model with multi-dimensional capabilities. The model can incorporate 3-D, 2-D laterally averaged, 2-D vertically averaged, and 1-D elements in a single grid. Wetting and drying of shallows is implemented.

Dimensionality: 3-D with multi-dimensional capabilities

Governing equations: Fully non-linear Reynolds form of Navier Stokes Equations with hydrostatic assumption
Continuity of Mass
Advection-Diffusion of Salt
Advection-Diffusion of Temperature
Equation of State

Turbulence sub-model:

Horizontal: Eddy viscosity

Vertical: Eddy viscosity with a variety of built-in functions for calculating or specifying eddy viscosity coefficients. The Mellor-Yamada second moment closure model is included as an option.

Time-stepping scheme:

Semi-implicit finite difference scheme (forward time centering at 62.5%).

Numerical solution technique:

Galerkin-finite element formulation in space

Newton-Raphson non-linear iteration scheme

"Front" matrix solver for sparse matrices

Type of grid: Unstructured, isoparametric finite element grid

3-D elements: bricks, tetrahedra, prisms, pyramids

2-D elements: quadrilaterals, triangles

1-D elements: lines

Coordinate transformations:

Horizontal: none

Vertical: z-transform

Example applications: Galveston Bay; San Francisco Bay; Cape Fear River, New York Harbor

Typical Δt for 3-D baroclinic circulation:

15 minutes to 1 hour

Reference: King, 1993

ESTUARINE HYDRODYNAMIC MODEL

Author(s): R. A. Luettich, Jr. and J. J. Westerink

Organization: University of North Carolina at Chapel Hill, Institute of Marine Sciences (Luettich), and

University of Notre Dame, Department of Civil Engineering (Westerink)

Contributors (modifications and enhancements):

Name of model: ADCIRC-3DL (Advanced three-dimensional circulation model, local)

Related models: ADCIRC-2DDI (2-D vertically averaged hydrodynamics)

ADCIRC-3DB (3-D baroclinic hydrodynamics, under development)

Remarks:

The local 3D model is a quasi 3-D model, in that lateral advection and diffusion is ignored in the internal mode. This approximation is only applicable when the rate of vertical momentum transport is much greater than the rate of horizontal momentum transport. This model is intended for use in coastal and shelf waters. Constant density is assumed in the 3DL model, although baroclinic terms are included in the 2-D vertically averaged (external) mode equations. A fully 3-D baroclinic version is under development.

Dimensionality: "Local" 3D

Governing equations: Vertically integrated generalized wave continuity equation (WCE) that is decoupled from the solution for vertically averaged velocity

Vertically integrated Reynolds form of Navier Stokes equations with hydrostatic

assumption, lateral turbulent diffusion optionally turned off

Simplified vertical momentum transport based on local approximation of the 3-D equations, i.e. advective terms and horizontal momentum diffusion are neglected in the 3-D equations and constant density assumed

Turbulence sub-model:

Horizontal: Eddy viscosity optionally turned on

Vertical: Direct Stress-Solution: solves for vertical shear stress distribution rather than velocity, based on vertically averaged solution

Time-stepping scheme: Split mode solution:

1. Three time level, variably weighted implicit finite difference for most terms of the WCE solution (vertically averaged, external mode)

2. Explicit approximation for non-linear and certain body force terms of WCE solution (vertically averaged, external mode)

3. Two time level, implicit Crank-Nicholson finite difference scheme for most terms of 2-D momentum equations (vertically averaged, external mode)

4. Explicit scheme for convective and bottom friction terms in 2-D momentum equations (vertically averaged, external mode)

5. Two-time level, implicit Crank-Nicholson scheme for simplified 3-D vertical stress equations (internal mode)

Numerical solution technique: Finite element

Type of grid: Unstructured finite element grid consisting of linear triangles and bi-linear quadrilaterals in the horizontal.

Coordinate transformations:

Horizontal: none

Vertical: σ-coordinate system

Example applications: Gulf of Mexico, Atlantic Ocean

Typical Δt for 3-D baroclinic circulation:

90 seconds

Reference: Luettich, Westerink and Scheffner, 1991

Luettich and Westerink, 1991

ESTUARINE HYDRODYNAMIC MODEL

Author(s): Ralph T. Cheng and Vincenzo Casulli

Organization: U.S. Geological Survey, Menlo Park, CA (Cheng), and

Istituo per le Applicazioni del Calcolo, Rome (Casulli)

Contributors (modifications and enhancements):

Name of model: TRIM-3D (Tidal, Residual, Intertidal Mudflat Model)

Related models: TRIM-2D (2-D vertically averaged hydrodynamics)

Remarks:

The TRIM codes are state-of-the-art finite difference codes. The programming style is extremely portable between computing platforms. There is little flexibility in the grid set-up, but high resolution grids can be applied at reasonable computational cost because of the fast alternating direction implicit (ADI) scheme. The Cartesian grid system is particularly well suited to open bays, lakes, and coastal regions.

The TRIM codes employ an Eulerian-Lagrangian scheme for the convection terms in both the momentum equations and in the advection-diffusion model. Wetting and drying of shallows is implemented. A corresponding cohesive sediment transport model is currently under development.

Dimensionality: 3-D, and automatically consistent with the 2-D vertically averaged equations when one vertical layer is specified.

Governing equations: Fully non-linear Reynolds form of Navier Stokes Equations with hydrostatic assumption
Continuity of Mass
Advection-Diffusion of Salt

Advection-Diffusion of Temperature
Equation of State

Turbulence sub-model:

Horizontal: Eddy viscosity

Vertical: Under development

Time-stepping scheme: Semi-implicit finite difference

Implicit discretization of the gradient of the surface elevation in the momentum equations and the velocity in the vertically integrated continuity equation.

Explicit discretization of the convective, turbulence and certain body force terms.

Numerical solution technique: Finite difference

Type of grid: Cartesian finite difference, constant grid spacing

Coordinate transformations:

Horizontal: none

Vertical: none

Example applications: San Francisco Bay; Lagoon of Venice

Typical Δt for 3-D baroclinic circulation:

1 to 2 minutes

Reference: Casulli and Cheng, 1992

Cheng, Casulli, and Gartner, 1993

ESTUARINE HYDRODYNAMIC MODEL

Author(s): Y. Peter Sheng / Billy H. Johnson

Organization: University of Florida, Gainesville, Florida /

USACE Waterways Experiment Station, Vicksburg, MS

Contributors (modifications and enhancements):

Name of model: CH3D (Curvilinear-Grid Hydrodynamic 3-D) /

CH3D-WES (WES version of CH3D)

Related models:

EHSM3D (Estuary Hydrodynamic and Sediment Model 3-D, Cartesian coordinates)

CH2D (Curvilinear-Grid Hydrodynamic 2-D Vertically Averaged)

Remarks:

Dr. Sheng continues to update and make enhancements to the model. Dr. Sheng has developed water quality/sediment transport models that interface with CH3D and EHSM3D.

WES has made significant modifications to the code that have resulted in a functionally separate version, CH3D-WES. The WES version has been modified to use either a σ-transform or a z-transform, dependent upon application. Wetting and drying is not implemented in the current WES version of the code. A water quality / aquatic ecology model has been developed to interface with CH3D-WES. A three-dimensional sediment transport model is currently under development for WES (anticipated completion date: October 1993).

Dimensionality: 3-D

Governing equations: Fully non-linear Reynolds form of Navier Stokes with hydrostatic approximation

Continuity of Mass

Advection-Diffusion of Salinity

Advection-Diffusion of Temperature

Equation of State

Turbulence sub-model:

Horizontal: Eddy viscosity

Vertical: Simplified second moment closure model

Time-stepping scheme: Split mode solution:

1. Semi-implicit finite difference for the external mode (vertically averaged) solution

2. All terms of the internal mode solution are treated explicitly, except for the vertical turbulent diffusion terms, and the bottom friction and surface slope terms in the momentum equations

Numerical solution technique: Finite difference

Type of grid: Curvilinear, staggered, boundary fitted, structured

Coordinate transformations:

Vertical: σ-coordinate system.

Horizontal: curvilinear, boundary fitted

Example applications: Lake Okeechobee; Sarasota Bay (Sheng)

Chesapeake Bay; Delaware Bay; Green Bay (WES)

Typical Δt for 3-D baroclinic circulation:

2 to 10 minutes

(Equal time steps are used for internal and external modes)

Reference: Sheng, 1993

Johnson, et al., 1991

Sheng, 1986

ESTUARINE HYDRODYNAMIC MODEL

Author(s): John E. Edinger and Edward M. Buchak

Organization: J. E. Edinger Associates, Inc., Wayne, Pennsylvania

Contributors (modifications and enhancements):

Name of model: GLLVHT5 (Generalized, Longitudinal-Lateral-Vertical Hydrodynamic and Transport Model, Version 5)

Related models:

Remarks: A description of this model is being prepared by Dr. Edinger. The description will be included in the WES publication of this report. The anticipated publication date is 1994.

Dimensionality: 3-D

Governing equations: **Turbulence sub-model:**

Horizontal:

Vertical:

Time-stepping scheme:

Numerical solution technique:

Type of grid:

Coordinate transformations:

Vertical:

Horizontal:

Example applications:

Typical Δt for 3-D baroclinic circulation:

Reference:

ESTUARINE HYDRODYNAMIC MODEL

Author(s): Di Hua Zhao, Guillermo Q. Tabios, Hsieh Wen Shen

Organization: University of California, Berkeley

Contributors (modifications and enhancements):

Name of model: RBFVM-2D

Related models: none

Remarks:

This model is included for review because it is the only published finite volume model currently being used for surface water flows. In its present form it is not applicable to stratified estuarine flow, however there is great potential for three-dimensional model development. The finite volume method has merit for shallow surface water flow problems because wetting and drying of sub-domains is handled naturally. An implicit version is being developed to alleviate the time step restriction.

Dimensionality: 2-D vertically averaged hydrodynamics

Governing equations: 2-dimensional shallow water equations with constant density

Turbulence sub-model:

Horizontal: neglected

Vertical: none

Time-stepping scheme: Explicit

Numerical solution technique: Finite volume method

Type of grid: Unstructured with quadrilateral and triangle elements

Coordinate transformations:

Horizontal: none

Vertical: none

Example applications: Kissimmee River Basin

Typical Δt for 2-D vertically averaged circulation:

less than one second

Reference: Zhao, Tabios, and Shen, 1992

7. RECOMMENDED CRITERIA FOR SELECTING A HYDRODYNAMIC/SALINITY MODEL FOR THE LSJRE

The State of Florida has tasked the SJRWMD to determine the ecological and water quality condition of the St. Johns River, and to develop management strategies that balance multiple beneficial uses of the river. Potential beneficial uses may include water supply, navigation, industrial and residential use of shorelines, domestic and industrial waste discharges, fisheries, wildlife habitat and recreation. From an engineering perspective, the objectives of the SJRWMD are

1. to understand the existing physical, chemical, and biological functions of the LSJRE;

2. to develop tools to scientifically predict the impacts of alternative management plans and engineering projects on the LSJRE; and

3. to develop a methodology for evaluating the costs and benefits of alternative management plans, based on predictions.

Numerical models have the potential for integrating basin-wide hydrodynamic and water quality data with scientific principals in a quantitative manner. Given the directive of the State of Florida to the SJRWMD, such sophisticated analysis tools are warranted.

The selection of a hydrodynamic model for the LSJRE is the first step in creating a comprehensive modeling and analysis system. The recommended features of a model that will meet the long range goals of the SJRWMD, and a brief justification of each feature, are given below:

1. MINIMUM DIMENSIONALITY: Two-dimensional, vertically averaged estuarine hydrodynamics

   The LSJRE includes approximately 110 miles of tidally influenced river channel. Although several one-dimensional models have been applied to the LSJRE, the process of verifying a one-dimensional model frequently results in unrealistic values for roughness, channel geometry, and water quality diffusion

coefficients. Two-dimensional, vertically averaged models have been found to require far less "tuning" to achieve satisfactory tidal simulations, and are more useful for making valid predictions.

The lower 100 miles of the St. Johns River varies from 600 feet to 1.5 miles nominal width (Morris, 1993). The wider reaches actually fluctuate between 1.5 and 3.0 miles in width, depending upon local flood conditions. A vertically averaged model will capture momentum losses due to expansions and contractions of the river channel, which affect the progression of tides and flood waves. Furthermore, lateral momentum transport occurring at junctions of the main stem with tributaries will be well represented. These characteristics are important for the ultimate computation of sediment transport and water quality, especially when the sediment load or water chemistry of the tributary is different from the main stem.

2. POTENTIAL DIMENSIONALITY: Three-dimensional, baroclinic hydrodynamics

The LSJRE has been categorized as a highly stratified to moderately stratified estuary (Morris, 1993). A salt wedge of variable extent has been reported in the LSJRE. Vertical stratification due to salinity or temperature gradients results in vertical velocity gradients and secondary circulation which can only be described by a three-dimensional model of estuarine hydrodynamics. Secondary currents can also result from flow around channel bends and from wind stress.

A three-dimensional model represents a substantial increase in sophistication over the two-dimensional, vertically averaged model. Certain modeling objectives, such as waste load allocation or flood routing, do not warrant three-dimensional analysis. However, if the model results are to be used for modeling salinity stratification and the response of phytoplankton to changing salinity, then a three-dimensional model will be required. A

prudent approach would be to select a two-dimensional, vertically averaged hydrodynamic model that has a three-dimensional counterpart either in existence or actively under development. Since most three-dimensional models are built upon a two-dimensional preliminary grid, the preparatory work of grid development, developing boundary conditions, and data gathering will carry over to three dimensions when the need for a three-dimensional study arises.

3. GEOMETRY: Boundary fitted grid with local refinement options

Because the St. Johns River is bathymetrically complex, it is important to define the complexities accurately. The scale of flow phenomena vary because of the dramatic changes in width and depth along the length of the river. Either a stretched, curvilinear, boundary fitted finite difference grid or an unstructured finite element grid (or finite volume grid) would be appropriate. A capability for rapid local refinement of the grid will be advantageous as new study areas are defined.

4. WETTING AND DRYING OPTION: Required

Portions of the St. Johns River and its tributaries are adjacent to tidal and freshwater marshes. Flooding and drying of marsh areas can have a significant impact on the volume of the tidal prism, the phasing of tidal fluctuations, and the storage volume of the estuary. As part of the LSJRE ecosystem, marshes may play an important role in filtering sediments and water quality, and provide habitat for fish and wildlife. A model of LSJRE hydrodynamics should be capable of handling intermittent flooding of marsh environments, or to represent marsh storage schematically.

5. HORIZONTAL TURBULENT FLUCTUATION TERMS: Required

Hydrodynamic circulation in the LSJRE is largely controlled by the complex geometry of the estuary. Boundary shear is important around expansions and contractions of the river,

islands, and river bends. Horizontal turbulent fluctuation terms are thus required to adequately simulate LSJRE flows. Wave equation models that ignore horizontal eddy viscosity are not appropriate for this system.

6. VERTICAL TURBULENT CLOSURE MODEL: Documentation Required

An advanced turbulence closure model such as the Mellor-Yamada scheme is recommended for the three-dimensional hydrodynamic model. A three-dimensional modeling study will only be useful if the model can capture the stratification behavior of the estuary. This behavior is generally controlled by the vertical turbulence model. The vertical turbulence closure scheme of the selected model should be well documented, including guidance for selecting values of the coefficients.

7. MODEL MAINTENANCE: Required

The models described in this paper are actively under development. The planning period for development of the SJRWMD modeling program is three to five years. It is desirable that the modeling tools developed under this program be useful and up to date for several years beyond the development program. Therefore, it is prudent to choose a modeling system that is designed to take advantage of new theoretical developments, and new computer technology. When contracting for modeling services, provision for model maintenance and upgradability should be negotiated.

Given the above requirements, several of the models reviewed in Chapter 4 can be considered most appropriate for the LSJRE system. These models are (in no particular order)

A. RMA-10 and associated models, Ian P. King / WES

B. CH3D, Y. P. Sheng / CH3D-WES, Y. P. Sheng and B. H. Johnson

C. ECOM, Alan F. Blumberg and George L. Mellor

Each of these models has strengths and weaknesses for the LSJRE application. For example, Model A is the only one of the three that has a fully implemented wetting and drying scheme. Models B and C can handle marshes schematically by adding "storage nodes". Model A is not currently linked to a water quality model that includes phytoplankton. Models B and C are each linked to an advanced water quality model.

Models A and B are public domain models that have been applied to various estuarine flow problems by the authors at their respective institutions. WES uses both of these models, the choice of which is made according to the requirements of the specific application. Model C is proprietary and is available by contract with the authors.

8. HYDRODYNAMIC MONITORING REQUIREMENTS TO SUPPORT MODEL OF LSJRE

Application of a hydrodynamic/salinity model to the LSJRE will require field data to set boundary conditions and to perform model verification. The minimum data requirements are summarized in the following table.

Data Category	Data Type	Sampling Locations	Sampling Frequency	Period of Record
Boundary Conditions and Initial Conditions	Tidal elevation	Two or three locations at the ocean boundary	2.0 -15.0 minutes	Continuous over spring-neap tidal sequence, plus long-term records from permanent tide stations (existing or to be established)
	Velocity or Discharge	Tributaries, point discharges, and upstream boundary	Daily	Continuous record of length determined by seasonality of tributary flows
	Salinity	Minimally 6 to 12 point measurements throughout the estuary (vertically resolved)	Daily	Short-term records (for initial conditions)
		Tributaries, point discharges, and upstream boundary	Daily	Continuous record of length determined by seasonality of tributary flows
		Two or three locations at ocean boundary (vertically resolved)	0.5 - 1.0 hours	Continuous over one spring-neap tidal sequence for each season

Data Category	Data Type	Sampling Locations	Sampling Frequency	Period of Record
Boundary Conditions and Initial Conditions	Temperature	Minimally 6 to 12 point measurements throughout the estuary (vertically resolved)	Daily	Short-term records (for initial conditions)
		Tributaries, point discharges, and upstream boundary	Daily	Continuous record of length determined by seasonality of tributary flows
		Two or three locations at ocean boundary (vertically resolved)	0.5 - 1.0 hours	Continuous over spring-neap tidal sequence
	Wind Speed and Direction	Point measurements throughout the estuary	Hourly	Continuous record of length determined by seasonality of local meteorology
Model Verification (Two or more independent data sets required).	Tidal elevation	Minimally 6 to 12 point measurements throughout the estuary and at ocean boundary	2.0 - 15.0 minutes	Continuous over spring-neap tidal sequence, plus long-term records from existing permanent tide stations
	Velocity	Minimally 6 to 12 point measurements throughout the estuary and at ocean boundary (vertically resolved)	2.0 - 15.0 minutes	Continuous over spring-neap tidal sequence

Data Category	Data Type	Sampling Locations	Sampling Frequency	Period of Record
Model Verification (Two or more independent data sets required).	Salinity	Minimally 6 to 12 point measurements throughout the estuary and at ocean boundary (vertically resolved)	0.5 - 1.0 hours	Continuous over spring-neap tidal sequence
	Temperature	Minimally 6 to 12 point measurements throughout the estuary and at ocean boundary (vertically resolved)	0.5 - 1.0 hours	Continuous over spring-neap tidal sequence

9. RECOMMENDED APPROACH FOR LSJRE MODEL DEVELOPMENT PROGRAM

The tasks required for development of a comprehensive modeling and monitoring system for the LSJRE are outlined below. An estimated timeline for accomplishing these tasks is also provided. The timeline estimates are hypothetical, dependent upon the satisfactory completion of preliminary tasks. Furthermore, the estimates for water quality and sediment modeling system development are subject to modification depending upon the development status of the selected model.

Hydrodynamic Model Development Program

H1. Develop detailed objectives and management goals for hydrodynamic model development program.

H2. Select hydrodynamic model and contract for license, model maintenance, and consulting services.

H3. Develop limited objectives for initial, two-dimensional vertically averaged hydrodynamic model application (time and space scales to be simulated, hydrologic conditions for verification, questions to be answered).

H4. Develop two-dimensional vertically averaged hydrodynamic grid based on existing maps and surveys.

H5. Obtain preliminary boundary condition data from historic record.

H6. Perform field reconnaissance to verify map details.

H7. Perform preliminary simulations.

H8. Compare model to historical data.

H9. Analyze and document preliminary results.

H10. Determine data deficiencies and inadequacies. Recommend additions/deletions in hydrodynamic monitoring network.

H11. Perform further model simulations. Continue to test against new data.

H12. Analyze and document secondary results.

H13. Develop plans for future two-dimensional, vertically averaged model applications. Determine if existing grid resolution, validation, and analysis system is adequate for future applications. Develop program of model maintenance and systematic application to support SJRWMD management objectives.

H14. Develop limited objectives for initial, three-dimensional hydrodynamic model application (time and space scales to be simulated, hydrologic conditions for verification, questions to be answered).

H15. Develop three-dimensional hydrodynamic grid.

H16. Develop three-dimensional boundary condition data.

H17. Perform preliminary simulations.

H18. Compare model to historical data.

H19. Analyze and document preliminary results.

H20. Determine data deficiencies and inadequacies. Recommend additions/deletions in hydrodynamic monitoring network.

H21. Perform further model simulations. Continue to test against new data.

H22. Analyze and document secondary results.

H23. Develop plans for future three-dimensional model applications. Determine if existing grid resolution, verification, and analysis system is adequate for future applications. Develop program of model maintenance, enhancement, and systematic application to support SJRWMD management objectives.

TIME LINE FOR HYDRODYNAMIC MODEL DEVELOPMENT PROGRAM

Task	YEAR 1	YEAR 2	YEAR 3	YEAR 4	YEAR 5
H1	-->				
H2	->				
H3	--->				
H4	---->				
H5	---->				
H6	---->				
H7	---->				
H8	---->				
H9	-----	---->			
H10	-----	---->			
H11		--------->			
H12		--------->			
H13	----------	----------	--------->		
H14	--->				
H15	--	-->			
H16		--------->			
H17		----------	-->		
H18		----------	-->		
H19		----------	-->		
H20			--------->		
H21			----------	--------->	
H22			----------	--------->	
H23		----------	----------	--------->	

Sediment Transport Model Development Program

S1. Develop detailed objectives and management goals for sediment transport model development program.

S2. Review sediment modeling literature.

S3. Select sediment model and contract for license, model maintenance, model interface development (if required) and consulting services.

S4. Develop limited objectives for initial, sediment model application (time and space scales to be simulated, conditions for verification, questions to be answered).

S5. Initiate/expand sediment monitoring program.

S6. Obtain sediment characterization and boundary condition data.

S7. Perform preliminary simulations.

S8. Compare model results to prototype to the extent possible with existing data.

S9. Analyze and document preliminary results.

S10. Determine data deficiencies and inadequacies. Recommend additions/deletions in sediment monitoring network.

S11. Perform further model simulations. Continue to test against new data.

S12. Analyze and document secondary results.

S13. Develop plans for future sediment dynamic model applications. Determine if existing grid resolution, verification, and analysis system is adequate for future applications. Develop program of model maintenance and systematic application to support SJRWMD management objectives.

TIME LINE FOR SEDIMENT MODEL DEVELOPMENT PROGRAM

Task	YEAR 1	YEAR 2	YEAR 3	YEAR 4	YEAR 5
S1	--------->				
S2	-----	-->			
S3		-->			
S4		---->			
S5	-----	----------	----------	----------	--------->
S6		--------->			
S7		--------	->		
S8		--------	->		
S9		--------	->		
S10		--------	->		
S11			----------	--------->	
S12			----------	--------->	
S13		--------	----------	----------	--------->

Water Quality Model Development Program

Q1. Develop detailed objectives and management goals for water quality model development program.

Q2. Review water quality modeling literature.

Q3. Select water quality model and contract for license, model maintenance, model interface development (if required) and consulting services.

Q4. Develop limited objectives for initial, water quality model application (time and space scales to be simulated, conditions for verification, questions to be answered).

Q5. Initiate/expand water quality monitoring program.

Q6. Obtain water quality boundary condition data.

Q7. Perform preliminary simulations.

Q8. Compare model to the extent possible with existing data.

Q9. Analyze and document preliminary results.

Q10. Determine data deficiencies and inadequacies. Recommend additions/deletions in water quality monitoring network.

Q11. Perform further model simulations. Continue to test against new data.

Q12. Analyze and document secondary results.

Q13. Develop plans for future water quality model applications. Determine if existing grid resolution, verification, and analysis system is adequate for future applications. Develop program of model maintenance and systematic application to support SJRWMD management objectives.

TIME LINE FOR WATER QUALITY MODEL DEVELOPMENT PROGRAM

Task	YEAR 1	YEAR 2	YEAR 3	YEAR 4	YEAR 5
Q1	----------	--------->			
Q2	-----	--------->			
Q3		--->			
Q4		----	->		
Q5	-----	----------	----------	----------	--------->
Q6		----	----->		
Q7			--------->		
Q8			--------->		
Q9			--------->		
Q10			--------->		
Q11			---	----------	--------->
Q12			---	----------	--------->
Q13		----	----------	----------	--------->

Hydrodynamic Monitoring Program Development

HM1. Determine gauge locations, sampling intervals, maintenance schedules for hydrodynamic data stations in consultation with modelers and end users.

HM2. Develop data base for hydrodynamic, sediment, and water quality field data analysis, storage, and retrieval.

HM3. Install gauges.

HM4. Collect and analyze data.

HM5. Review procedures; coordinate with modeling team; revise program as needed.

Sediment Monitoring Program Development

SM1. Determine parameters, procedures, gauge locations, sampling intervals, maintenance schedules for sediment data stations.

SM2. Expand and maintain data base for hydrodynamic and water quality field data analysis, storage, and retrieval.

SM3. Obtain samplers and equipment if required.

SM4. Collect and analyze data..

SM5. Review procedures; coordinate with modeling team; revise program as needed.

Water Quality Monitoring Program Development

QM1. Determine parameters, procedures, gauge locations, sampling intervals, maintenance schedules for water quality data stations.

QM2. Expand and maintain data base for hydrodynamic and water quality field data analysis, storage, and retrieval.

QM3. Obtain samplers and equipment if required.

QM4. Collect and analyze data..

QM5. Review procedures; coordinate with modeling team; revise program as needed.

TIME LINE FOR DEVELOPMENT OF MONITORING PROGRAM

Task	YEAR 1	YEAR 2	YEAR 3	YEAR 4	YEAR 5
HM1	----->				
HM2	----------	---->			
HM3	------->				
HM4	--------	----------	----------	----------	--------->
HM5	----	----------	----------	----------	--------->
SM1	----	--->			
SM2	----	--------->			
SM3	----	----->			
SM4	--	----------	----------	----------	--------->
SM5	--	----------	----------	----------	--------->
QM1	----	--->			
QM2	----	--------->			
QM3	----	----->			
QM4	--	----------	----------	----------	--------->
QM5	--	----------	----------	----------	--------->

10. COMPUTER HARDWARE REQUIREMENTS

Two-dimensional, vertically averaged models for estuarine hydrodynamics are currently being run on mini-computers and mid-size workstations. The cost of cpu and memory in this class of machines has steadily decreased over the past several years and this trend is expected to continue. Turn around times for workstation batch jobs rival the speeds of shared resource computers because the new chips are extremely fast and the user has local control over job processing. The advantages of a workstation environment include:

a. graphical user interface,

b. moderate initial cost,

c. personal control of job schedules, and

d. multi-tasking.

Three-dimensional models are computationally very expensive and time consuming. Current run times for fully non-linear 3-D estuarine models running on mini-computers are typically about one-half of real time, depending on the size of the grid and the solution technique. Super-computers such as the CRAY Y-MP are used for long-term 3-D simulations. However, workstation cpu power is gaining rapidly on the super-computer market. Low-end, multi-processor machines are also being developed which can take advantage of vectorizable codes. With these advancements, a locally owned, powerful workstation with periodic upgrades is likely to be the most cost efficient solution for estuarine modeling. At the current rate of workstation development, an evaluation of computer resources and equipment upgrade is recommended every other year.

In addition to the cpu, the following equipment and software are required:

Digitizer

Graphics monitor

FORTRAN Compiler

C Compiler

Plotting software

High quality printer for graphics

Mass data storage device

11. GRAPHICAL USER INTERFACE

Estuarine models require a great deal of spatial and time varying data. The models generate three-dimensional time series of the hydrodynamic, sediment transport, and water quality parameters. A graphical user interface is necessary to organize information, to analyze results, and to gain a physical understanding of the processes described by these data. The graphical interface should be designed to manage model I/O, visualize three-dimensional data, and facilitate model development and applications. Several graphical user interfaces have been developed specifically for handling data sets arising from geophysical flow models. A graphical user interface may be purchased from a third party vendor or as part of the model license. As with other components of the modeling software, a contract for software maintenance and updates is recommended.

12. COSTS

The cost of developing a comprehensive estuarine flow model is difficult to estimate. Costs are proportional to the degree of sophistication required to answer specific management questions. The following figures illustrate "ball park" figures for a small scale model development plan using existing codes. The costs cited do not include development of new codes, interfaces, or modeling technologies that may be required to address certain complex problems. The projected costs are based on a time table of model development similar to that described in Section 8. More elaborate plans will increase program costs.

Costs for implementing the hydrodynamic, water quality and sediment monitoring programs are not included in these estimates. It is assumed that field programs will be conducted by local agencies, and therefore must be budgeted according to local labor and equipment resources. A comprehensive modeling program simply will not succeed without coordination between the monitoring program and the modeling program. The monitoring costs cited in this table reflect the efforts of the modeling team to coordinate the field effort, and special reconnaissance related specifically to modeling needs.

System Component	Estimated Cost				
	YEAR 1	YEAR 2	YEAR 3	YEAR 4	YEAR 5
Hydrodynamic Modeling System	$100,000	$100,000	$50,000	$10,000	
Sediment Transport Modeling System	$10,000	$100,000	$100,000	$50,000	$10,000
Water Quality Modeling System	$10,000	$50,000	$100,000	$100,000	$50,000
Computer Equipment Purchase and Maintenance	$50,000	$10,000	$10,000	$30,000	$10,000
Graphical User Interface	$20,000	$20,000	$10,000	$10,000	$10,000
Oversee Hydrodynamic Monitoring Program	$20,000	$20,000	$20,000	$20,000	$20,000
Oversee Sediment Monitoring Program	$20,000	$50,000	$50,000	$20,000	$20,000
Oversee Water Quality Monitoring Program	$20,000	$50,000	$50,000	$20,000	$20,000
TOTAL	$250,000	$400,000	$390,000	$260,000	$140,000

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Section B

Review of Water Quality Monitoring and Recommendations for Water Quality Modeling of the Lower St. Johns River

Review of Water Quality Monitoring and Recommendations for Water Quality Modeling of the Lower St. Johns River

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Report prepared for the Jacksonville District, USACE and the St. Johns River Water Management District

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Introduction

The St. Johns River Water Management District (SJRWMD) has plans to develop a comprehensive modeling system for the Lower St. Johns River Estuary (LSJRE). The modeling system will be used to provide information for issues concerning watershed management, water supply, pollutant loadings, and eutrophication. Thus, the modeling system will require models of the watershed, hydrodynamics, sediment transport processes, and water quality including algal/nutrient/dissolved oxygen interactions and contaminants. The water quality model is an important component of the system. In light of this, the SJWRMD has requested a review of the present water quality monitoring program to insure that proper and sufficient data are being collected to support future water quality modeling efforts.

This report reviews present water quality data gathering efforts, recommends additional data efforts, and recommends and discusses a water quality model suitable to meet the objectives of the SJRWMD.

Water Quality Monitoring

Data provided by SJRWMD for review were limited in scope. These data included a list of parameters presently sampled by the SJRWMD, sampling station locations used by SJRWMD and other agencies, values of typical water quality parameters plotted spatially from just downstream of the Ocklawaha River to the estuary mouth for one sampling event, and average values from 1983 to 1992 for three sections of the St. Johns River. Therefore, a comprehensive review of existing data is not possible in this report. The following provides a limited discussion of the provided water quality data and discusses in general terms water quality data requirements necessary to support a water quality model of the LSJR.

Existing Monitoring

Sampled Parameters

Table 1 lists the parameters routinely sampled for by SJRWMD. In addition, metals including calcium, magnesium, chromium, zinc, lead, cadmium, and copper are also monitored.

Spatial Monitoring

The SJRWMD has an extensive water quality sampling program in place. Information provided by SJRWMD shows that approximately 40 stations are routinely sampled throughout the Lower St. Johns River by the SJRWMD. Approximately 50 additional stations are sampled by other agencies. No information was supplied as to what water quality parameters were sampled at the additional stations. Major tributaries appear to be adequately represented allowing for development of river loading estimates. No information was provided on the vertical extent of sampling.

Temporal Monitoring

Water quality parameters are typically sampled once a month. In addition, synoptic sampling events the length of the lower river are conducted approximately twice a year. No information was provided as to what parameters are sampled for during the synoptic events. It is assumed that the parameters include those listed in Table 1.

Determination of Loadings

A key to any successfull water quality modeling effort is an accurate determination of the loadings to the system. Without the correct loadings, calibration of the model is difficult and results of management scenarios will be suspect at best. It is therefore crucial to obtain accurate loading estimates. Stations at tributary mouths are presently sampled monthly. This is not sufficient to determine accurate

Table 1
Sampled Water Quality Parameters

Parameter	Frequency
Temperature	monthly
pH	monthly
Dissolved oxygen	monthly
Ammonium-N	monthly
Nitrate + Nitrite-N	monthly
Total Kjeldahl N	monthly
Total phosphorus	monthly
Orthophosphate	monthly
Dissolved silica	monthly
Total suspended solids	monthly
Total dissolved solids	monthly
Sulfate	monthly
Chloride	monthly
Chlorophyll A,B,C, and phaephyton	monthly
Total organic carbon	monthly
Alkalinity	monthly
Turbidity	monthly
Color	monthly

estimates of tributary loadings. A sampling procedure for estimating loads from tributary loads will be discussed in more detail in the next section.

Recommended Water Quality Monitoring

Table 2 lists the recommended parameters necessary for supporting a state-of-the-art water quality model of the Lower St. Johns River. Of primary importance are particulate (POC) and dissolved organic carbon (DOC), primary production, and sediment oxygen demand and nutrient fluxes. Dissolved organic carbon plays a key role in eutrophication related issues in the LSJR. Based on color measurements and visual inspection of the LSJR, it appears that productivity in the fresh water portion

of the river is limited by light penetration due primarily to DOC. Discussions with personnel from SJRWMD suggest that loadings of DOC are primarily from major tributaries and wetland areas in the upper portion of the river. Therefore, it is imperative that accurate regressions of DOC with flow be developed for estimating DOC loadings to the system. Total inorganic carbon, along with pH and alkalinity, will allow modeling of the pH-carbonate system.

Also of importance are determinations of phytoplankton productivity and respiration rates and bioassays for nutrient limitations. Water quality models are capable of computing nutrient and light limitations and bioassays would be helpful in comparing model predictions. Productivity and respiration rates are necessary for accurate characterization of carbon assimilation by phytoplankton.

It is also critical to obtain accurate estimates of sediment oxygen demand and nutrient fluxes for proper calibration of a sediment model or for proper specification of boundary values if a sediment model is not used. In addition, proper characterization of the sediments including particulate organic carbon, phosphorus, nitrogen, and inorganic phosphorus is necessary for sediment model calibration.

Total carbon, nitrogen, phosphorus, and silica are necessary to insure that loadings during model calibration are correctly accounted for. Care should be taken during analysis so that no single component is greater than the total nutrient. If this occurs, samples should be immediately analyzed again.

Monthly sampling frequency for all in-pool parameters is generally sufficient in the early stages of a sampling program. However, as knowledge of the system behavior increases, sampling frequency during the most dynamic periods may have to be increased to better capture the dynamics of the system. For example, it may be necessary to sample more frequently during shifts in phytoplankton assemblages in order to gain a better understanding of phytoplankton succession. It is critical to have an understanding of the system in order to accurately represent the processes during a modeling effort. In addition, most modeling studies give direction to future sampling efforts by pinpointing deficiences in the existing data.

Concerning contaminant modeling, it is hard to make specific recommendations without knowing the contaminant of concern. However, the following parameters should be measured for any contaminant modeling study. In the sediments, bulk and dry density, grain size, TOC and DOC, longterm burial velocities, and contaminant concentrations should be measured. Longterm burial rates are typically determined from strontium core datings. In the water column, total and dissolved contaminant concentrations, TOC and DOC, and settling velocity should be measured. In addition, sorption and degradation values should be determined from either the literature or from laboratory experiments.

Table 2
Recommended Monitoring Parameters

Water Column	
Temperature	Dissolved phosphate
Salinity	Particulate inorganic phosphorus*
Light extinction	Dissolved organic phosphorus*
Dissolved oxygen	Particulate organic phosphorus*
Ammonium	Total phosphorus*
Nitrate_nitrite	Dissolved silica
Dissolved organic nitrogen*	Particulate biogenic silica*
Particulate organic nitrogen*	Total silica*
Total Nitrogen*	Chlorophyll
pH	Total inorganic carbon*
Alkalinity	
Sediments	
Particulate organic carbon*	Particulate inorganic phosphorus*
Particulate organic nitrogen*	Particulate organic phosphorus*
Processes/Fluxes	
Primary production*	Sediment nitrate flux*
Respiration*	Sediment phosphorus flux*
Sediment oxygen demand*	Sediment silica flux*
Sediment ammonium flux*	Sediment COD flux*
Nutrient limitation bioassays*	

* recommended additional sampling and analyses

Water Quality Modeling

Recommended Water Quality Model

The recognized state-of-the-art water quality model with respect to eutrophication related issues is CE-QUAL-ICM (Cerco and Cole, 1993). The model is similar in concept to WASP (Ambrose, et.al., 1986) and was developed over the last six years by the Water Quality and Contaminant Modeling Branch at Waterways Experiment Station for application to Chesapeake Bay. The model is presently being used by the U.S. Army Engineer Waterways Experiment Station (WES) to evaluate the effectiveness of nutrient reduction strategies on eutrophication in the Bay, and has also been used to address management issues in the New York Bight, Indian River-Reheboth Bay, Delaware, LA Long Beach, and Lower Green Bay. CE-QUAL-ICM is the first 3-D water quality model shown to be capable of addressing water quality issues spanning multiple decades.

Capabilities

Mass Balance

Water quality modeling can be viewed simply as mass-balance modeling wherein the model keeps track of constituent mass over time as it is affected by external boundary conditions and internal kinetic transformations. CE-QUAL-ICM has been shown to account for constituent mass within the accuracy of a given computer. This is the most fundamental requirement of any water quality model - the water quality transformations and numerical solution scheme must maintain mass balances.

Hydrodynamic Linkage

CE-QUAL-ICM is a finite-volume model. Theoretically, the model can link to hydrodynamic models of any dimension or combination of dimensions using either structured or unstructured grids. However, certain numerical solution techniques in the model complicate the linkage to unstructured grid, hydrodynamic models. This will be discussed in more detail in the **Limitations** section.

Transport

CE-QUAL-ICM is a stand alone water quality code decoupled from the hydrodynamics. Output, specifically flows and diffusivities across cell faces, from a chosen hydrodynamic model is used to drive the transport processes. Diffusivities can be optionally specified in the water quality model. The model is capable of addressing long-term water quality issues in one, two, or three dimensions, or in any combination. Thus, a variety of hydrodynamic models can be used to provide transport information required by CE-QUAL-ICM.

A major advancement incorporated in the model is a subcomponent which calculates residual currents from the hydrodynamic model averaged over a given time period (typically a tidal cycle). This allows

for longer timesteps in the water quality model while still maintaining the transport properties of the hydrodynamic model and contributes to the model's ability to perform longterm simulations. The calculation of residual currents is presently incorporated into the hydrodynamic model CH3D (Dortch, 1992). Additional effort would be required to provide residual flows from a different hydrodynamic model.

Another important advancement incorporated into CE-QUAL-ICM is a higher-order numerical transport scheme, QUICKEST (Leonard, 1979), which greatly reduces numerical diffusion during constituent transport. It is well known that upwind differencing produces numerical dispersion which can often be much greater than the physical dispersion. Because of numerical dispersion, upwind differencing cannot resolve sharp gradients which are typically encountered when modeling water quality. The transport solution scheme in CE-QUAL-ICM can use either upwind differencing or QUICKEST. The preferred method is QUICKEST. The Chesapeake Bay Study showed that observed vertical gradients in salinity could not be reproduced in the hydrodynamic model without the inclusion of a higher-order transport scheme (Johnson, 1991).

Vertical transport is differentiated from horizontal transport in the model. Vertical diffusion is always handled implicitly in time which removes vertical diffusion from numerical stability criteria. Vertical advection employs a time-weighted scheme which can vary between fully explicit, fully implicit, or a combination of the two. The fully implicit option also eliminates vertical advection from the transport stability criteria. The combination of fully implicit vertical advection and diffusion contributes to the model's ability to conduct longterm simulations (ie., decades) required when evaluating nutrient reduction scenarios or contaminant modeling.

The model also includes an algorithm which adjusts the timestep based on estimates of numerical stability criteria required by the numerical solution of the advection-diffusion equation. Thus, the timestep automatically decreases during periods of high constituent fluxes and increases during low periods. Previously, the timestep in most water quality models was set to the lowest value encountered during a simulation in order to maintain numerical stability. Automatic model adjustment of the timestep is referred to as autostepping and has a dramatic effect on reducing the computational requirements of the model.

Eutrophication Interactions

The model contains a full suite of water quality constituents used to address eutrophication related issues. A complete description of the state variables and their interactions is given in Appendix A. This appendix is provided primarily to allow the reader to determine if the important processes and proper formulations for the LSJR are included in the model. This appendix was taken from a draft report of the Chesapeake Bay study (Cerco and Cole, 1993).

Sediment Submodel

CE-QUAL-ICM contains a predictive sediment submodel which represents the accumulation and decay or diagenisis of organic matter in the sediments and its effect on water column oxygen demand and nutrient fluxes from the sediments (DiToro and Fitzpatrick, 1993). The present sediment formulation is applicable mainly to saline conditions in the water column. A freshwater formulation which includes iron and manganese will be incorporated into the model in the future.

Limitations

It was previously stated that CE-QUAL-ICM is the state-of-the-art in water quality modeling. However, it does not contain all of the state-of-the-art capabilities available today in the field of water quality modeling. It should be noted that no other water quality model contains complete state-of-the-art capabilities either. The model was initially developed to address specific management issues for the Chesapeake Bay Study, but the coding of the model is such that additional capabilities can be incorporated as needed. In addition, the algorithms in the code are applicable but not specific to Chesapeake Bay.

Experience has shown that nearly every new application of any water quality model requires inclusion of additional processes or reformulation of existing processes in order to adequately reproduce prototype behavior. CE-QUAL-ICM will evolve over time as new applications require additional capabilities or reformulations. The most important limitations of the model are discussed below.

Hydrodynamic Linkage

The only hydrodynamic model used to drive the transport processes in previous CE-QUAL-ICM applications is CH3D-WES (Johnson, 1991). CH3D-WES is discussed in the companion report and will be discussed only briefly in this report. The discretization grid is boundary fitted, curvilinear, structured, and space staggered. The vertical grid can be either sigma-stretched where the number of layers in the grid are fixed and layer thicknesses vary temporally throughout the water column, or a Z-grid representation where only the surface layer varies in thickness over time. CE-QUAL-ICM is capable of linking to either vertical grid. Most importantly, the higher-order transport scheme in CE-QUAL-ICM requires a structured grid representation. CH3D meets this requirement.

Theoretically, finite-element hydrodynamic models using unstructured grids can be used to drive the transport processes in CE-QUAL-ICM. However, finite-element, unstructured grids have not previously been used with CE-QUAL-ICM. Plans have been made to incorporate the ability to link CE-QUAL-ICM to unstructured grids, but it must be emphasized that research would be involved in linking the water quality model to a finite-element, hydrodynamic model. The following considerations are involved with linking CE-QUAL-ICM to a finite-element hydrodynamic model.

Finite-element hydrodynamic models conserve mass globally, but do not conserve mass locally. As stated previously, the fundamental principle in water quality modeling involves keeping track of constituent mass through external boundary interactions and internal kinetic transformations. Presently, it is not known what affect the inability of a hydrodynamic model to locally conserve mass will have on the ability of CE-QUAL-ICM to reproduce behavior in the prototype. It is believed that finite-element hydrodynamic models can be corrected to conserve mass locally, but, as stated previously, research would be required to establish this.

More importantly, the present higher-order transport scheme (QUICKEST) in CE-QUAL-ICM requires three spatial points to interpolate constituent fluxes across cell faces. Linking CE-QUAL-ICM to an unstructured hydrodynamic model would require the development of a two-point, higher-order transport scheme since the three points required by the present scheme would not be readily discernable. Such schemes are available, but again, research would be involved in implementing the two-point, higher-

order transport scheme. Additionally, the new transport scheme must be shown to reproduce the transportive properties of the hydrodynamic solution scheme.

Future Capabilities

Numerous improvements to CE-QUAL-ICM are planned in the future. They are discussed in the following sections.

Sediment Submodel w/ Iron and Manganese Kinetics

The current sediment model was developed to compute carbon diagenesis and sediment-water column fluxes for Chesapeake Bay which is predominately saltwater. Development is underway to make the sediment submodel applicable to freshwater sediments. The main differences between the freshwater and saltwater formulations are that sulfides are the primary source of oxygen demand in saltwater and methane, iron, and manganese along with sulfides are the primary sources of sediment oxygen demand in freshwater.

Carbonate-pH System

A carbonate-pH system with non-conservative alkalinity is being incorporated into the model. A fully tested system is expected by 1995.

Zooplankton

The initial water quality formulations in CE-QUAL-ICM explicitly included the effects of zooplankton by their inclusion as state variables. During model calibration, zooplankton were removed from the formulations and their effects were included in the algal mortality and nutrient recycling terms. Plans are to reintroduce zooplankton into the model as state variables for Phase 2 of the Chesapeake Bay Study.

Macrophytes

Macrophyte/nutrient interactions are not presently included in CE-QUAL-ICM. Phase 2 of the Chesapeake Bay Study will incorporate macrophytes as a state variable. This is presently an active area of research in the modeling community and improvements will be incorporated in the future as a better understanding of the processes are gained.

Contaminants

The contaminant components of the EPA's WASP model (Ambrose, et. al.,1986) are presently being incorporated into the model. No contaminant studies have been conducted with CE-QUAL-ICM; however, a water quality and contaminant modeling study of San Diego Bay is scheduled to start in 1994.

Sediment Transport

Sediment transport is presently not in the model. It should be relatively easy to incorporate sediment transport given sediment transport output from an appropriate hydrodynamic model. Again, sediment transport will probably be incorporated into the model during the San Diego Bay study.

Pre- and Postprocessors

One of the most serious shortcomings of CE-QUAL-ICM is a lack of integrated pre- and postprocessors. Presently, the development of input files requires a hodgepodge of FORTRAN programs whose workings are largely undocumented. The same is true for postprocessing of output. Graphical display of model output consists of a series of FORTRAN programs which use high level graphics subroutine calls from a commercial package called DISSPLA. There are plans to develop integrated processors based on a graphical user interface. However, given the current level of funding, development will take several years to complete.

Computer Requirements

Hardware

CE-QUAL-ICM has previously been run on 80386/80486 PC's, RISC workstations, and a Cray Y-MP and C-90. All of the code developement for Chesapeake Bay was performed on a 25 Mhz 80386 PC while model calibration and scenario runs were performed on a Cray Y-MP. Given the rapid advancements in the state-of-the-art in hardware for computationally intensive floating-point code, it is hard to estimate future hardware requirements for management scenarios. It is almost a certainty that the model will run in a reasonable time on workstations costing less than 10K in five years.

Software

Present software requirements are a FORTRAN compiler and a commercial software package called DISSPLA for processing of model output. For PC's, the compiler must be capable of addressing 32-bits in DOS's protected mode. The trend in workstations is toward 64-bit CPU's which deliver the same precision as Cray supercomputers. Machines with 64-bits of precision are not a requirement of the model, but they increase the accuracy of the computations.

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Appendix A
CE-QUAL-ICM Kinetic Formulations

The central issues in the water quality model are primary production of carbon by algae and dissolved oxygen concentrations. Primary production provides the energy required by the ecosystem to function. Excessive primary production is detrimental since its decomposition in the water and sediments consumes oxygen. Dissolved oxygen is necessary to support the life functions of higher organisms and is considered an indicator of the "health" of estuarine systems. In order to predict primary production and dissolved oxygen, a large suite of model state variables is necessary (Table A-1).

Table A-1
Water Quality Model State Variables

Temperature	Salinity
Total Active Metal	Cyanobacteria
Diatoms	Green Algae
Dissolved Organic Carbon	Labile Particulate Organic Carbon
Refractory Particulate Organic Carbon	Ammonium
Nitrate	Dissolved Organic Nitrogen
Labile Particulate Organic Nitrogen	Refractory Particulate Organic Nitrogen
Total Phosphate	Dissolved Organic Phosphorus
Labile Particulate Organic Phosphorus	Refractory Particulate Organic Phosphorus
Chemical Oxygen Demand	Dissolved Oxygen
Particulate Biogenic Silica	Available Silica

Conservation Of Mass Equation

The foundation of CE-QUAL-ICM is the solution to the three-dimensional mass-conservation equation for a control volume. The control-volume approach was selected to allow maximum flexibility in linking CE-QUAL-ICM to alternate hydrodynamic models. For each state variable, the conservation of mass is:

$$\frac{\delta V_i C_i}{\delta t} = \sum_{j=1}^{n} Q_j C_j^* + \sum_{j=1}^{n} A_j D_j \frac{\delta C}{\delta x_j} + \sum S_i \qquad \text{(A-1)}$$

where

V_i = volume (m^3)
C_i = concentration (g m^{-3})
Q_j = volumetric flow across flow face j (m^3 sec^{-1})
C^*_j = concentration in flow across flow face j (g m^{-3})
A_j = area of flow face j (m^2)
D_j = diffusion coefficient at flow face j (m^2 sec^{-1})
n = number of flow faces attached to control volume
S_i = external loads and kinetic sources and sinks in control volume (g sec^{-1})
t, x = temporal and spatial coordinates

Solution to the mass-conservation equation uses the QUICKEST finite difference algorithm (Leonard 1979) for horizontal advection and diffusion and a Crank-Nicolson scheme for vertical advection and diffusion.

State Variables

Algae

Algae are grouped into three model classes: cyanobacteria, diatoms, and greens. The grouping is based upon the distinctive characteristics of each class and upon the significant role they play in the ecosystem. Cyanobacteria, commonly called blue-green algae, are characterized by their abundance (as picoplankton) in saline water and by their bloom-forming characteristics in fresh water. Cyanobacteria are unique in that some species fix atmospheric nitrogen. The cyanobacteria in the model are bloom--forming species that do not fix nitrogen. They are characterized as having negligible settling velocity and subject to low predation pressure. Diatoms are distinguished by their requirement of silica as a nutrient to form cell walls with high settling velocities. Settling of spring diatom blooms to the sediments may be a significant source of carbon for sediment oxygen demand. Algae that do not fall into the preceding two groups are lumped into the heading of green algae. Green algae settle at a rate intermediate between cyanobacteria and diatoms and are subject to greater grazing pressure than cyanobacteria.

Organic Carbon

Three organic carbon state variables are included: dissolved, labile particulate, and refractory particulate. Labile and refractory distinctions are based upon the time scale of decomposition. Labile organic

carbon decomposes on a time scale of days to weeks while refractory organic carbon requires more time. Labile organic carbon decomposes rapidly in the water column or the sediments. Refractory organic carbon decomposes slowly, primarily in the sediments, and contributes to sediment oxygen demand years after deposition.

Nitrogen

Nitrogen is divided into organic and mineral fractions. Organic nitrogen state variables are: dissolved organic nitrogen, labile particulate organic nitrogen, and refractory particulate organic nitrogen. Two mineral nitrogen forms are modeled - ammonium and nitrate/nitrite. Both forms are available for algal nutrient requirements although ammonium is preferred from thermodynamic considerations. The primary reason for distinguishing the two is that ammonium is oxidized by nitrifying bacteria into nitrate. This oxidation can be a significant sink of oxygen in the water column and sediments. An intermediate in the complete oxidation of ammonium, nitrite, also exists. Nitrite concentrations are usually much less than nitrate and, for modeling purposes, are combined with nitrate. The nitrate state variable represents the sum of nitrate plus nitrite.

Phosphorus

As with carbon and nitrogen, organic phosphorus is considered in three states: dissolved, labile particulate, and refractory particulate. Only a single mineral form, total phosphate, is considered. Total phosphate exists in several states within the model: dissolved phosphate, phosphate sorbed to inorganic solids, and phosphate incorporated in algal cells. Equilibrium partition coefficients are used to distribute the total among the three states.

Silica

Silica is divided into two state variables: available silica and particulate biogenic silica. Available silica is primarily dissolved and can be used by diatoms. Particulate biogenic silica cannot be used. In the model, particulate biogenic silica is produced through diatom mortality. Particulate biogenic silica undergoes dissolution to available silica or settles to the bottom sediments.

Chemical Oxygen Demand

Chemical oxygen demand is modeled as the concentration of reduced substances that are oxidizable by inorganic means. The primary component of chemical oxygen demand is sulfide released from sediments. Oxidation of sulfide to sulfate may remove substantial quantities of dissolved oxygen from the water column.

Dissolved Oxygen

Dissolved oxygen is required for the existence of higher life forms. Oxygen availability determines the distribution of organisms and the flow of energy and nutrients in an ecosystem. Dissolved oxygen is a central component of the water quality model.

Total Active Metal

Both phosphate and dissolved silica sorb to inorganic solids - primarily iron and manganese. Sorption and subsequent settling is one pathway for removal of phosphate and silica from the water column. The sediment model does not include iron and manganese. Instead, total active metal is defined as the total concentration of metals that are active in phosphate and silica adsorption and transport. Total active metal is partitioned between particulate and dissolved phases by an oxygen-dependent partition coefficient.

Salinity

Salinity is a conservative tracer that provides verification of the transport component of the model and facilitates examination of conservation of mass. Salinity also influences the dissolved oxygen saturation concentration and is used in the determination of kinetics constants that differ in saline and fresh water.

Temperature

Biochemical reactions are a function of temperature. Reaction rates increase with increasing temperature. Extreme temperatures cause algal mortality.

Kinetic Formulations

The remainder of this appendix details the kinetics of the mass-conservation equation for each state variable. Parameters are defined where they first appear. For consistency with reported rate coefficients, kinetic reactions are defined with a temporal dimension of days. Within the CE-QUAL-ICM code, kinetics sources and sinks rates are converted to seconds for the mass-conservation equation.

Algae

Algae play a central role in the carbon and nutrient cycles. Equations governing the three algal groups are similar with differences among groups expressed through the magnitudes of coefficients in the

equations. The letter "x" is used as a "wild card" in the equations and is replaced with a letter that indicates a specific algal group. Algal groups are indicated by:

c = cyanobacteria
d = diatoms
g = green algae

Sources and sinks of algae are:

Growth (production)
Basal metabolism
Predation
Settling

The governing equation for algal biomass is:

$$\frac{\delta}{\delta t} Bx = \left[Px - BMx - PRx - WSx \frac{\delta}{\delta z} \right] Bx \qquad \text{(A-2)}$$

where

Bx = algal biomass, expressed as carbon (g C m^{-3})
Px = production (day^{-1})
BMx = basal metabolism (day^{-1})
PRx = predation (day^{-1})
WSx = settling velocity (m day^{-1})
z = vertical coordinate (m)

Production

Production by phytoplankton is determined by nutrient availabilty, light intensity, and temperature. The effects are considered to be multiplicative:

$$Px = PMx\, f(N)\, f(I)\, f(T) \qquad \text{(A-3)}$$

where

PMx = production under optimal conditions (day^{-1})
f(N) = effect of suboptimal nutrient concentration ($0 \leq f \leq 1$)
f(I) = effect of suboptimal illumination ($0 \leq f \leq 1$)
f(T) = effect of suboptimal temperature ($0 \leq f \leq 1$)

Cyanobacteria are treated as freshwater organisms that undergo rapid mortality in salt water. This effect is included by a salinity toxicity term in the cyanobacteria production equation:

$$Pc = PMc\ f(N)\ f(I)\ f(T)\ f(S) \tag{A-4}$$

where

f(S) = effect of salinity on cyanobacteria production ($0 \leq f \leq 1$)

Nutrients

Carbon, nitrogen, and phosphorus are the primary nutrients required for algal growth. Diatoms also require silica. Inorganic carbon limitation is not considered in the model. The effects of the remaining nutrients on growth are described by Monod kinetics (Monod 1949). In this formulation, growth is dependent upon nutrient availability at low nutrient concentrations but is independent of nutrients at high concentrations. A key parameter in the formulation is the half-saturation concentration. In this formulation, the growth rate is half the maximum when available nutrient concentration equals the half-saturation concentration. Liebig's "law of the minimum" (Odum 1971) states that growth is determined by the nutrient in least supply. For cyanobacteria and greens:

$$f(N) = \text{minimum}\left\{\frac{NH_4 + NO_3}{KHnx + NH_4 + NO_3}, \frac{PO_4d}{KHpx + PO_4d}\right\} \tag{A-5}$$

where

NH4 = ammonium concentration (g N m^{-3})
NO3 = nitrate concentration (g N m^{-3})
KHnx = half-saturation constant for nitrogen uptake (g N m^{-3})
PO_4d = dissolved phosphate concentration (g P m^{-3})
KHpx = half-saturation constant for phosphorus uptake (g P m^{-3})

Some cyanobacteria, notably the bloom-forming genus *Anabaena*, utilize atmospheric nitrogen to supply nitrogen requirements. In the model, a non-nitrogen fixing algae is considered the predominant cyanobacteria. The potential growth of nitrogen fixers, such as *Anabaena*, can be estimated by removing the nitrogen limitation on cyanobacteria.

Diatoms require silica as well as nitrogen and phosphorus for growth. For diatoms, the nutrient limitation is the minimum of the limitations expressed in Equation A-5 or the following:

$$f(N) = \frac{SAd}{KHs + SAd} \qquad \text{(A-6)}$$

where

SAd = dissolved available silica concentration (g Si m^{-3})
KHs = half-saturation constant for silica uptake by diatoms (g Si m^{-3})

Light

Algal production increases as a function of light intensity until an optimal intensity is reached. Beyond the optimal intensity, production declines as intensity increases. Steele's equation (DiToro et al. 1971) describes this phenomenon:

$$f(I) = \frac{I}{Is} e^{1 - \frac{I}{Is}} \qquad \text{(A-7)}$$

where

I = illumination rate (Langleys day^{-1})
Is = optimal illumination (Langleys day^{-1})

Steele's equation describes the instantaneous light limitation at a point in space. However, the model computes limitation integrated over discrete time intervals and aggregated spatially by model segments. In the model, Steele's equation is integrated over one day and is averaged over the thickness of each model segment. This interval does not preclude computation steps less than a day but frees the model from accounting for illumination in "real time." Daily averaging precludes computation of diurnal fluctuations in algal production. This restriction is not severe since the equations for algal growth are not appropriate for short time scales.

Assuming light intensity declines exponentially with depth, the integrated, averaged form of Steele's equation is:

$$f(I) = \frac{2.72\,FD}{Kess\,\Delta z}\left(e^{\alpha b} - e^{\alpha t}\right) \qquad \text{(A-8)}$$

$$\alpha b = -\frac{Io}{FD\,Is} e^{-Kess(ZD + \Delta z)} \qquad \text{(A-9)}$$

$$\alpha t = - \frac{Io}{FD\, Is} e^{- Kess\, ZD} \qquad (A\text{-}10)$$

where

Io = daily illumination at water surface (Langleys day^{-1})
FD = fractional daylength ($0 \leq FD \leq 1$)
Kess = total light attenuation coefficient (m^{-1})
Δz = model segment thickness (m)
ZD = distance from water surface to top of model segment (m)

Light attenuation in the water column is composed of two fractions: a background value dependent on water color and concentration of suspended particles, and extinction due to light absorption by chlorophyll:

$$Kess = Keb + Kechl \sum_{x=c,d,g} \frac{1}{CChlx} Bx \qquad (A\text{-}11)$$

where

Keb = background light attenuation (m^{-1})
Kechl = light attenuation coefficient for chlorophyll 'a' ($m^2\ mg^{-1}$)
CChlx = carbon-to-chlorophyll ratio of algal group x (g C mg^{-1} chl)

Optimal illumination for photosynthesis depends on algal taxonomy, duration of exposure, temperature, nutrient status, and previous acclimation. Variations in optimal illumination are largely due to adaptations by algae intended to maximize production in a variable environment. Steele (1962) noted the result of adaptations is that optimal illumination is a consistent fraction ($\simeq$ 50%) of daily illumination. Kremer and Nixon (1978) reported an analogous finding that maximum algal production occurs at a constant depth ($\simeq$ 1m) in the water column. Their approach is adopted here so that optimal illumination is expressed:

$$Isx = Ioavg\, e^{- Kess\, Doptx} \qquad (A\text{-}12)$$

where

Ioavg = adjusted surface illumination (Langleys day^{-1})
Doptx = depth of maximum algal production (m)

A minimum, Ismin, is specified for optimal illumination so that algae do not thrive at extremely low light levels. The time required for algae to adapt to changes in illumination is accounted for by computing Is based on a time-weighted average of daily illumination:

$$Ioavg = 0.7\,Io + 0.2\,I1 + 0.1\,I2 \qquad \text{(A-13)}$$

where

I1 = daily illumination one day preceding model day (Langleys day^{-1})
I2 = daily illumination two days preceding model day (Langleys day^{-1})

Temperature

Algal production increases as a function of temperature until an optimum temperature is reached. Above the optimum, production declines until a lethal temperature is reached. Numerous functional representations of temperature effects are available. Inspection of growth versus temperature curves indicates a function similar to a Gaussian probability curve provides a good fit to observations:

$$f(T) = e^{-KTgx1\,(T - Tmx)^2} \text{ when } T \leq Tmx$$
$$= e^{-KTgx2\,(Tmx - T)^2} \text{ when } T > Tmx \qquad \text{(A-14)}$$

where

T = temperature (C^o)
Tmx = optimal temperature for algal growth (C^o)
KTgx1 = effect of temperature below TMx on growth ($C^{o\,-2}$)
KTgx2 = effect of temperature above TMx on growth ($C^{o\,-2}$)

Salinity Toxicity

The effect of salinity on freshwater cyanobacteria is represented by an empirical equation:

$$f(S) = \frac{Stox^2}{Stox^2 + S^2} \qquad \text{(A-15)}$$

where

Stox = salinity which Microcystis growth is halved (ppt)

Settling

In late winter and early spring, diatom populations are assumed to be characterized by large species with high settling velocities. At the end of spring, large diatoms are assumed to be replaced by populations of smaller individuals with lower settling velocities. Diatom settling is represented in the model as:

$$WSd = WSdb + Prdval\,WSds \quad \text{(A-16)}$$

where

WSdb = base diatom settling velocity (m day^{-1})
WSds = enhanced settling velocity of large diatoms (m day^{-1})
Prdval = piecewise function used to specify seasonal diatom settling velocity

Basal Metabolism

In the model, basal metabolism is the sum of all internal processes that decrease algal biomass. A portion of metabolism is respiration which may be viewed as a reversal of production. In respiration, carbon and nutrients are returned to the environment accompanied by the consumption of dissolved oxygen. A second internal sink of biomass is the excretion of dissolved organic carbon.

Respiration cannot proceed in the absence of oxygen. Basal metabolism cannot decrease in proportion to oxygen availability or algae would approach immortality under anoxic conditions. To solve this dilemma, basal metabolism is considered to be independent of dissolved oxygen concentration but the distribution of metabolism between respiration and excretion is oxygen-dependent. When oxygen is freely available, respiration is a large fraction of the total. When oxygen is restricted, excretion becomes dominant. Formulation of this process is detailed in the text that describes algal effects on carbon and dissolved oxygen.

Basal metabolism is commonly considered to be an exponentially increasing function of temperature:

$$BMx = BMrx\, e^{KTbx\,(T\,-\,Trx)} \quad \text{(A-17)}$$

where

BMrx = metabolic rate at Trx (day^{-1})
KTbx = effect of temperature on metabolism ($C^{o\,-1}$)
Trx = reference temperature for metabolism (C^{o})

Predation

Detailed specification of predation rates requires predictive modeling of zooplankton biomass and activity. At present, zooplankton are not included in the model. Consequently, a constant predation rate is specified. The present formulation assumes zooplankton biomass is a constant fraction of algal biomass. Zooplankton activity is assumed to be influenced by temperature and is taken into account by incorporating an exponential temperature relationship into the predation term. The predation formula-

tion is identical to basal metabolism. The difference in predation and basal metabolism lies in the distribution of the end products of these processes:

$$PRx = BPRx\, e^{KTbx(T - Trx)} \qquad \text{(A-18)}$$

where

BPRx = predation rate at Trx (day^{-1})

Effect of Algae on Organic Carbon

During production and respiration, algae primarily take up and produce carbon dioxide, an inorganic form not considered in the model. A small fraction of basal metabolism is exuded as dissolved organic carbon. In the model, this fraction increases as dissolved oxygen becomes scarce. Algae also produce organic carbon through the effects of predation. Zooplankton take up and redistribute algal carbon through grazing, assimilation, respiration, and excretion. Since zooplankton are not included in the model, routing of algal carbon through zooplankton is simulated by empirical distribution coefficients. The effects of algae on organic carbon are expressed as:

$$\frac{\delta}{\delta t} DOC = \left[\left[FCDx + (1 - FCDx) \frac{KHrx}{KHrx + DO} \right] BMx + FCDP\, PRx \right] Bx \qquad \text{(A-19)}$$

$$\frac{\delta}{\delta t} LPOC = FCLP\, PRx\, Bx \qquad \text{(A-20)}$$

$$\frac{\delta}{\delta t} RPOC = FCRP\, PRx\, Bx \qquad \text{(A-21)}$$

where

DOC = dissolved organic carbon concentration (g C m^{-3})
DO = dissolved oxygen concentration (g O_2 m^{-3})
LPOC = labile particulate organic carbon concentration (g C m^{-3})
RPOC = refractory particulate organic carbon concentration (g C m^{-3})
FCDx = fraction of basal metabolism exuded as dissolved organic carbon
KHrx = half-saturation concentration for algal dissolved organic carbon excretion (g O_2 m^{-3})
FCDP = fraction of dissolved organic carbon produced by predation
FCLP = fraction of labile particulate carbon produced by predation
FCRP = fraction of refractory particulate carbon produced by predation

The sum of the three predation fractions must equal unity.

Effect of Algae on Phosphorus

Algae take up dissolved phosphate during production and release dissolved phosphate and organic phosphorus through mortality. As with carbon, the fate of algal phosphorus released by metabolism and predation is represented by distribution coefficients. Since the total phosphate state variable includes both intra- and extracellular phosphate, no explicit representation of the effects of algae on phosphate is necessary. Distribution of total phosphate is determined by partition coefficients as detailed in the "PHOSPHORUS" section of this appendix. The equations that express the effects of algae on organic phosphorus are:

$$\frac{\delta}{\delta t} DOP = (BMx\ FPDx + PRx\ FPDP)\ APC\ Bx \qquad (A\text{-}22)$$

$$\frac{\delta}{\delta t} LPOP = (BMx\ FPLx + PRx\ FPLP)\ APC\ Bx \qquad (A\text{-}23)$$

$$\frac{\delta}{\delta t} RPOP = (BMx\ FPRx + PRx\ FPRP)\ APC\ Bx \qquad (A\text{-}24)$$

where

DOP = dissolved organic phosphorus concentration (g P m^{-3})
LPOP = labile particulate organic phosphorus concentration (g P m^{-3})
RPOP = refractory particulate organic phosphorus concentration (g P m^{-3})
APC = phosphorus-to-carbon ratio of all algal groups (g P g^{-1} C)
FPDx = fraction of dissolved organic phosphorus produced by metabolism
FPLx = fraction of labile particulate phosphorus produced by metabolism
FPRx = fraction of refractory particulate phosphorus produced by metabolism
FPDP = fraction of dissolved organic phosphorus produced by predation
FPLP = fraction of labile particulate phosphorus produced by predation
FPRP = fraction of refractory particulate phosphorus produced by predation

The sums of the metabolism and respiration fractions must each be less than or equal to unity.

Effect of Algae on Nitrogen

Algae take up ammonium and nitrate during production and release ammonium and organic nitrogen through mortality. Nitrate is internally reduced to ammonium before biomass synthesis occurs (Parsons et al. 1984). Trace concentrations of ammonium inhibit nitrate reduction so that, in the presence of ammonium and nitrate, ammonium is utilized first. The preference of algae for ammonium can be expressed empirically (Thomann and Fitzpatrick 1982):

$$PNx = NH_4 \frac{NO_3}{(KHnx + NH_4)(KHnx + NO_3)} + NH_4 \frac{KHnx}{(NH_4 + NO_3)(KHnx + NO_3)} \quad \text{(A-25)}$$

where

PNx = algal preference for ammonium uptake ($0 \leq PNx \leq 1$)

The ammonium preference function has two limiting values. When nitrate is absent, the preference for ammonium is unity. When ammonium is absent, the preference is zero. In the presence of ammonium and nitrate, the preference depends on the abundance of both forms relative to the half-saturation constant for nitrogen uptake. When both ammonium and nitrate are abundant, the preference for ammonium approaches unity. When ammonium is scarce but nitrate is abundant, the preference decreases in magnitude and a significant fraction of algal nitrogen comes from nitrate.

Algal nitrogen releases by metabolism and predation are represented by distribution coefficients. The effects of algae on the nitrogen state variables are expressed as:

$$\frac{\delta}{\delta t} NH_4 = (BMx\ FNIx + PRx\ FNIP - PNx\ Px)\ ANCx\ Bx \quad \text{(A-26)}$$

$$\frac{\delta}{\delta t} NO_3 = (PNx - 1)\ Px\ ANCx\ Bx \quad \text{(A-27)}$$

$$\frac{\delta}{\delta t} DON = (BMx\ FNDx + PRx\ FNDP)\ ANCx\ Bx \quad \text{(A-28)}$$

$$\frac{\delta}{\delta t} LPON = (BMx\ FNLx + PRx\ FNLP)\ ANCx\ Bx \quad \text{(A-29)}$$

$$\frac{\delta}{\delta t} RPON = (BMx\ FNRx + PRx\ FNRP)\ ANCx\ Bx \quad \text{(A-30)}$$

where

DON = dissolved organic nitrogen concentration (g N m^{-3})
LPON = labile particulate organic nitrogen concentration (g N m^{-3})

RPON = refractory particulate organic nitrogen concentration (g N m^{-3})
ANCx = nitrogen-to-carbon ratio of algae (g N g^{-1} C)
FNIx = fraction of inorganic nitrogen produced by metabolism
FNDx = fraction of dissolved organic nitrogen produced by metabolism
FNLx = fraction of labile particulate nitrogen produced by metabolism
FNRx = fraction of refractory particulate nitrogen produced by metabolism
FNIP = fraction of inorganic nitrogen produced by predation
FNDP = fraction of dissolved organic nitrogen produced by predation
FNLP = fraction of labile particulate nitrogen produced by predation
FNRP = fraction of refractory particulate nitrogen produced by predation

The sums of the metabolism fractions and the predation fractions must each equal unity.

Algal Stoichiometry

Algal biomass is quantified in units of carbon. In order to express the effects of algae on nitrogen and phosphorus, the ratios of nitrogen-to-carbon and phosphorus-to-carbon in algal biomass must be specified. Global mean values of these ratios are well known (Redfield et al. 1966). Algal composition is known to vary as a function of nutrient availability. As nitrogen and phosphorus become scarce, algae adjust their composition so that smaller quantities of these nutrients are required to produce carbonaceous biomass (Droop 1973; DiToro 1980; Parsons et al. 1984). The ratio is described by an empirical approximation:

$$APC = \frac{1}{PCprm1 + PCprm2\, e^{-PCprm3\, PO_4d}} \qquad \text{(A-31)}$$

where

PCprm1 = minimum carbon-to-phosphorus ratio (g C g^{-1} P)
PCprm2 = difference between minimum and maximum carbon-to-phosphorus ratio (g C g^{-1} P)
PCprm3 = effect of dissolved phosphate concentration on carbon-to-phosphorus ratio (m^3 g^{-1} P)

Effect of Algae on Dissolved Oxygen

Algae produce oxygen during photosynthesis and consume oxygen through respiration. The quantity produced depends on the form of nitrogen utilized for growth. More oxygen is produced, per unit of carbon fixed, when nitrate is the algal nitrogen source than when ammonium is the source. Equations describing algal uptake of carbon and nitrogen and production of dissolved oxygen (Morel 1983) are:

When ammonium is the nitrogen source, one mole of oxygen is produced per mole of carbon dioxide fixed. When nitrate is the nitrogen source, 1.3 moles oxygen are produced per mole of carbon dioxide fixed.

$$106\,CO_2 + 16\,NH_4^+ + H_2PO_4^- + 106\,H_2O \rightarrow \text{protoplasm} + 106\,O_2 + 15\,H^+ \quad \text{(A-32)}$$

$$106\,CO_2 + 16\,NO_3^- + H_2PO_4^- + 122\,H_2O + 17\,H^+ \rightarrow \text{protoplasm} + 138\,O_2 \quad \text{(A-33)}$$

The equation that describes the effect of algae on dissolved oxygen is:

$$\frac{\delta}{\delta t} DO = \left[(1.3 - 0.3\,PNx)\,Px - \frac{DO}{KHrx + DO} BMx \right] AOCR\,Bx \quad \text{(A-34)}$$

where

AOCR = dissolved oxygen-to-carbon ratio in respiration (2.67 g O_2 g^{-1} C)

The magnitude of AOCR is derived from a simple representation of the respiration process:

$$CH_2O + O_2 = CO_2 + H_2O \quad \text{(A-35)}$$

The quantity (1.3 - 0.3 PNx) is the photosynthesis ratio and expresses the molar quantity of oxygen produced per mole of carbon fixed. The photosynthesis ratio approaches unity as the algal preference for ammonium approaches unity.

Organic Carbon

Organic carbon undergoes numerous transformations in the water column. The model carbon cycle consists of the following:

Phytoplankton production
Phytoplankton exudation
Predation on phytoplankton
Dissolution of particulate carbon
Heterotrophic respiration
Denitrification
Settling

Algal production is the primary carbon source although carbon also enters the system through external loadings. Predation of algae releases particulate and dissolved organic carbon to the water column. A fraction of the particulate organic carbon undergoes first-order dissolution to dissolved organic carbon.

The remainder settles to the sediments. Dissolved organic carbon produced by phytoplankton exudation, predation, and dissolution is respired or denitrified as a first-order rate. No carbon is recycled from the sediments to the water column although oxygen demand created by carbon diagenesis is included in the model.

Dissolution and Respiration Rates

Dissolution and respiration rates depend on the availability of carbonaceous substrate and on heterotrophic activity. Heterotrophic activity and biomass have been correlated with algal activity and biomass across a wide range of natural systems (Bird and Kalff 1984; Cole et al. 1988). Consequently, algal biomass can be incorporated into dissolution and respiration rate formulations as a surrogate for heterotrophic activity. The correlation between algae and heterotrophs occurs because algae produce labile carbon that fuel heterotrophic activity. Dissolution and respiration processes do not require the presence of algae and may be fueled entirely by external carbon inputs. Representation of dissolution and respiration in the model allows specification of algal-dependent and algal-independent rates:

$$Kdoc = Kdc + Kdcalg \sum_{x=c,d,g} Bx \qquad \text{(A-36)}$$

where

Kdoc = respiration rate of dissolved organic carbon (day^{-1})
Kdc = minimum respiration rate (day^{-1})
Kdcalg = constant that relates respiration to algal biomass ($m^3\ g^{-1}\ C\ day^{-1}$)

$$Klpoc = Klc + Klcalg \sum_{x=c,d,g} Bx \qquad \text{(A-37)}$$

where

Klpoc = dissolution rate of labile particulate organic carbon (day^{-1})
Klc = minimum dissolution rate (day^{-1})
Klcalg = constant that relates dissolution to algal biomass ($m^3\ g^{-1}\ C\ day^{-1}$)

$$Krpoc = Krc + Krcalg \sum_{x=c,d,g} Bx \qquad \text{(A-38)}$$

where

Krpoc = dissolution rate of refractory particulate organic carbon (day^{-1})
Krc = minimum dissolution rate (day^{-1})
Krcalg = constant that relates dissolution to algal biomass ($m^3\ g^{-1}\ C\ day^{-1}$)

An exponential function relates dissolution and respiration to temperature.

Denitrification

As oxygen is depleted from natural systems, oxidation of organic matter is effected by the reduction of alternate oxidants (referred to as "alternate electron acceptors"). The sequence in which alternate acceptors are employed is determined by the thermodynamics of oxidation-reduction reactions. The first substance reduced in the absence of oxygen is nitrate. A representation of the denitrification reaction can be obtained by balancing standard half-cell redox reactions (Stumm and Morgan 1981):

$$4\,NO_3^- + 4\,H^+ + 5\,CH_2O \rightarrow 2\,N_2 + 7\,H_2O + 5\,CO_2 \qquad \text{(A-39)}$$

Equation A-39 describes the stoichiometry of the denitrification reaction. The kinetics in the model are first-order. The dissolved organic carbon respiration rate, Kdoc, is modified so that significant decay via denitrification occurs only when nitrate is freely available and dissolved oxygen is depleted. A parameter is included so that the anoxic respiration rate is slower than oxic respiration:

$$\text{Denit} = \frac{\text{KHodoc}}{\text{KHodoc} + \text{DO}} \frac{\text{NO}_3}{\text{KHndn} + \text{NO}_3} \text{AANOX Kdoc} \qquad \text{(A-40)}$$

where

Denit = denitrification rate of dissolved organic carbon (day^{-1})
AANOX = ratio of denitrification to oxic carbon respiration rate ($0 \leq \text{AANOX} \leq 1$)
KHodoc = half-saturation concentration of dissolved oxygen required for oxic respiration ($g\ O_2\ m^{-3}$)
KHndn = half-saturation concentration of nitrate required for denitrification ($g\ N\ m^{-3}$)

An exponential function relates denitrification to temperature. Parameter values in the function are the same as for dissolved organic carbon respiration.

Dissolved Organic Carbon

The complete representation of all dissolved organic carbon sources and sinks in the model is given by:

$$\frac{\delta}{\delta t}\text{DOC} = \sum_{x=c,d,g} \left(\left[\text{FCDx} + (1 - \text{FCDx}) \frac{\text{KHrx}}{\text{KHrx} + \text{DO}} \right] \text{BMx} + \text{FCDP PRx} \right] \text{Bx} \qquad \text{(A-41)}$$
$$+ \text{Klpoc LPOC} + \text{Krpoc RPOC} - \frac{\text{DO}}{\text{KHodoc} + \text{DO}} \text{Kdoc DOC} - \text{Denit DOC}$$

Labile Particulate Organic Carbon

The complete representation of all labile particulate organic carbon sources and sinks in the model ecosystem is given by:

$$\frac{\delta}{\delta t} \text{LPOC} = \sum_{x=c,d,g} \text{FCLP PRx Bx} - \text{Klpoc LPOC} - \text{WSl} \frac{\delta}{\delta z} \text{LPOC} \qquad \text{(A-42)}$$

where

WSl = settling velocity of labile particles (m day^{-1})

Refractory Particulate Organic Carbon

The complete representation of all refractory particulate organic carbon sources and sinks in the model ecosystem is given by:

$$\frac{\delta}{\delta t} \text{RPOC} = \sum_{x=c,d,g} \text{FCRP PRx Bx} - \text{Krpoc RPOC} - \text{WSr} \frac{\delta}{\delta z} \text{RPOC} \qquad \text{(A-43)}$$

where

WSr = settling velocity of labile particles (m day^{-1})

Phosphorus

The model phosphorus cycle includes the following processes:

Algal production and metabolism
Predation
Hydrolysis of particulate organic phosphorus
Mineralization of dissolved organic phosphorus
Settling
Exchange with inorganic solids

External loads provide the ultimate source of phosphorus to the system. Dissolved phosphate is incorporated by algae during growth and released as phosphate and organic phosphorus through respiration and predation. A portion of the particulate organic phosphorus hydrolyzes to dissolved organic phosphorus. The balance settles to the sediments. Dissolved organic phosphorus is mineralized to phosphate. A portion of the phosphate sorbs to inorganic solids and settles to the sediments. Within

the sediments, particulate phosphorus is mineralized and recycled to the water column as dissolved phosphate.

Effects on phosphorus of algal production, metabolism, and predation have already been detailed. Descriptions of hydrolysis and mineralization and of the total phosphate system follow.

Hydrolysis and Mineralization

In the model, hydrolysis is defined as the process by which particulate organic substances are converted to dissolved organic form. Mineralization is defined as the process by which dissolved organic substances are converted to dissolved inorganic form. Conversion of particulate organic phosphorus to phosphate proceeds through hydrolysis and mineralization. Direct mineralization of particulate organic phosphorus does not occur.

Mineralization of organic phosphorus is mediated by the release of nucleotidase and phosphatase enzymes by bacteria (Ammerman and Azam 1985; Chrost and Overbeck 1987) and algae (Matavulj and Flint 1987; Chrost and Overbeck 1987; Boni et al. 1989). Since the algae themselves release the enzyme and since bacterial abundance is related to algal biomass, the rate of organic phosphorus mineralization in the model is related to algal biomass. A remarkable property of the enzyme process is that alkaline phosphatase activity is inversely proportional to phosphate concentration (Chrost and Overbeck 1987; Boni et al. 1989). Put in different terms, when phosphate is scarce, algae stimulate production of an enzyme that mineralizes organic phosphorus to phosphate. This phenomenon is simulated by relating mineralization to the algal phosphorus nutrient limitation. Mineralization is highest when algae are strongly phosphorus limited and is least when no limitation occurs.

Expressions for mineralization and hydrolysis rates are:

$$Kdop = Kdp + \frac{KHp}{KHp + PO_4d} Kdpalg \sum_{x=c,d,g} Bx \qquad (A\text{-}44)$$

where

Kdop = mineralization rate of dissolved organic phosphorus (day^{-1})
Kdp = minimum mineralization rate (day^{-1})
KHp = mean half-saturation constant for algal phosphorus uptake (g P m^{-3})
= (KHpc + KHpd + KHpg)/3
Kdpalg = constant that relates mineralization to algal biomass (m^3 g^{-1} C day^{-1})

$$Klpop = Klp + \frac{KHp}{KHp + PO_4d} Klpalg \sum_{x=c,d,g} Bx \qquad (A\text{-}45)$$

where

Klpop = hydrolysis rate of labile particulate phosphorus (day^{-1})
Klp = minimum hydrolysis rate (day^{-1})
Klpalg = constant that relates hydrolysis to algal biomass ($m^3\ g^{-1}\ C\ day^{-1}$)

$$Krpop = Krp + \frac{KHp}{KHp + PO_4d} Krpalg \sum_{x=c,d,g} Bx \qquad (A\text{-}46)$$

where

Krpop = hydrolysis rate of refractory particulate phosphorus (day^{-1})
Krp = minimum hydrolysis rate (day^{-1})
Krpalg = constant that relates hydrolysis to algal biomass ($m^3\ g^{-1}\ C\ day^{-1}$)

An exponential function relates mineralization and hydrolysis rates to temperature.

When the nutrient concentration greatly exceeds the half-saturation concentration for algal uptake, the rate roughly equals the minimum. Algal biomass has little influence. As phosphorus becomes scarce relative to the half-saturation concentration, the rate increases. The magnitude of increase depends on algal biomass.

The Total Phosphate System

One fraction of total phosphorus in the water column is phosphorus incorporated in algal biomass. This fraction is computed in the model as the product of algal biomass and APC, the phosphorus-to-carbon ratio. In the environment, algae adjust their phosphorus content in response to external conditions. Algal phosphorus content is high when external phosphorus is abundant and phosphorus content is low when phosphorus is scarce. The adaptation of algae to their environment indicates the phosphorus-to-carbon ratio should be a variable in the model. However, treatment of the ratio as a variable greatly complicates computation of phosphorus transport due to the mixture of algal masses of different composition. The complication is avoided if intracellular and extracellular phosphorus are treated and transported as a single state variable. Intracellular and extracellular concentrations are determined by equilibrium partitioning of their sum.

Adsorption is the process in which ions or molecules are attracted to the surface of a solid. Phosphate ions exhibit a strong adsorption to particulate species of metals including iron and manganese. Particulate and dissolved fractions are determined by equilibrium partitioning of their sum.

The model phosphate state variable is defined as the sum of dissolved phosphate, sorbed phosphate, and algal phosphorus content as:

$$PO_4t = PO_4d + PO_4p + PO_4a \quad \text{(A-47)}$$

where

PO_4t = total phosphate (g P m^{-3})
PO_4d = dissolved phosphate (g P m^{-3})
PO_4p = particulate (sorbed) phosphate (g P m^{-3})
PO_4a = algal phosphorus (g P m^{-3})

Exchange With Particulate Metals

Detailed treatment of iron and manganese is not included in the model. Instead, the state variable total active metal is defined as the sum of all metals that act as sorption sites. Phosphate sorbs only to the particulate fraction of the total metal. Therefore, the total metal is partitioned into particulate and dissolved fractions via an equilibrium partition coefficient. Extracellular phosphate is partitioned by a linear sorption isotherm so that dissolved and particulate fractions are computed as:

$$PO_4d = \frac{1}{1 + Kadpo4\ TAMp} (PO_4t - PO_4a) \quad \text{(A-48)}$$

$$PO_4p = \frac{Kadpo4\ TAMp}{1 + Kadpo4\ TAMp} (PO_4t - PO_4a) \quad \text{(A-49)}$$

where

Kadpo4 = partition coefficient of sorbed vs. dissolved phosphate (m^3 mol^{-1})
TAMp = particulate total active metal (mol m^{-3})

Computation of Algal Phosphorus

Algal phosphorus is defined as:

$$PO_4a = APC \sum_{x=c,d,g} Bx \quad \text{(A-50)}$$

The phosphorus-to-carbon ratio is calculated by the empirical function expressed in Equation A-31.

The equations 4-31, A-48, A-49, A-50, form an implicit system. The implicit nature of the system can be seen by substituting the expressions for dissolved phosphate (Equation A-48) and algal phosphate (Equation A-50) into the expression for phosphorus-to-carbon ratio (Equation A-31):

$$APC = \frac{1}{PCprm1 + PCprm2\, e^{-PCprm3\,(PO_4a - APC \sum Bx)}} \qquad (A\text{-}51)$$

The phosphorus-to-carbon ratio appears on both sides of the equation and cannot be obtained explicitly. (For simplicity, Kadpo4 = 0 in this example.) Within the model code, the phosphorus-to-carbon ratio is obtained by iterative solution of Equation A-51 in each control volume. From the phosphorus-to-carbon ratio, algal phosphorus is computed (Equation A-50). Next, extra-cellular phosphate is partitioned into dissolved and particulate fractions (Eqs. A-48 and A-49).

Phosphate

Once the interactions of dissolved, particulate, and algal phosphate are made explicit, the balance of the equations describing phosphorus are straightforward summations of previously-described sources and sinks:

$$\frac{\delta}{\delta t} PO_4t = - \sum_{x=c,d,g} WSx \frac{\delta}{\delta z} APC\, Bx - WSs \frac{\delta}{\delta z} PO_4p + Kdop\, DOP \qquad (A\text{-}52)$$

where

WSs = settling velocity of particulate metal (m day^{-1})

Algal uptake and release of phosphate represents an exchange of phosphate fractions rather than a phosphate source or sink. Consequently, no algal source or sink terms are included in the phosphate mass-conservation equation. The settling terms are required to represent the settling of particulate phosphate incorporated in algal biomass or sorbed to particles.

Dissolved Organic Phosphorus

$$\frac{\delta}{\delta t} DOP = \sum_{x=c,d,g} (BMx\, FPDx + PRx\, FPDP)\, APC\, Bx + Klpop\, LPOP + Krpop\, RPOP - Kdop\, DOP \qquad (A\text{-}53)$$

Labile Particulate Organic Phosphorus

$$\frac{\delta}{\delta t} LPOP = \sum_{x=c,d,g} (BMx\ FPLx + PRx\ FPLP)\ APC\ Bx - Klpop\ LPOP - WSl \frac{\delta}{\delta z} LPOP \quad \text{(A-54)}$$

Refractory Particulate Organic Phosphorus

$$\frac{\delta}{\delta t} RPOP = \sum_{x=c,d,g} (BMx\ FPRx + PRx\ FPRP)\ APC\ Bx - Krpop\ RPOP - WSr \frac{\delta}{\delta z} RPOP \quad \text{(A-55)}$$

Nitrogen

The model nitrogen cycle includes the following processes:

Algal production and metabolism
Predation
Hydrolysis of particulate organic nitrogen
Mineralization of dissolved organic nitrogen
Settling
Nitrification
Denitrification

External loads provide the ultimate source of nitrogen to the system. Inorganic nitrogen is incorporated by algae during growth and released as ammonium and organic nitrogen through respiration and predation. A portion of the particulate organic nitrogen hydrolyzes to dissolved organic nitrogen. The balance settles to the sediments. Dissolved organic nitrogen is mineralized to ammonium. In an oxygenated water column, a fraction of the ammonium is subsequently oxidized to nitrate. In anoxic water, nitrate is lost to nitrogen gas through denitrification. Particulate nitrogen that settles to the sediments is mineralized and recycled to the water column, primarily as ammonium. Nitrate moves in both directions across the sediment-water interface, depending on relative concentrations in the water column and sediment interstices.

Effects on nitrogen of algal production, metabolism, and predation have already been detailed. Descriptions of hydrolysis, mineralization, nitrification and denitrification follow.

Hydrolysis and Mineralization

In the model, particulate organic nitrogen is converted to dissolved organic nitrogen via hydrolysis. Dissolved organic nitrogen is converted to ammonium through mineralization. Conversion of particulate nitrogen to ammonium proceeds through hydrolysis and mineralization. Direct mineralization of particulate nitrogen does not occur. The argument for accelerated hydrolysis and mineralization during nutrient-limited conditions is not as clear for nitrogen as for phosphorus. However, the same formulations are made available for nitrogen as for phosphorus. Accelerated processes can be activated or deactivated through parameter selection. The nitrogen hydrolysis and mineralization formulations are:

$$Kdon = Kdn + \frac{KHn}{KHn + NH_4 + NO_3} Kdnalg \sum_{x=c,d,g} Bx \qquad \text{(A-56)}$$

where

Kdon = mineralization rate of dissolved organic nitrogen (day^{-1})
Kdn = minimum mineralization rate (day^{-1})
KHn = mean half-saturation constant for algal nitrogen uptake (g N m^{-3})
= (KHnc + KHnd + KHng)/3
Kdnalg = constant that relates mineralization to algal biomass (m^3 g^{-1} C day^{-1})

$$Klpon = Kln + \frac{KHn}{KHn + NH_4 + NO_3} Klnalg \sum_{x=c,d,g} Bx \qquad \text{(A-57)}$$

where

Klpon = hydrolysis rate of labile particulate nitrogen (day^{-1})
Kln = minimum hydrolysis rate (day^{-1})
Klnalg = constant that relates hydrolysis to algal biomass (m^3 g^{-1} C day^{-1})

$$Krpon = Krn + \frac{KHn}{KHn + NH_4 + NO_3} Krnalg \sum_{x=c,d,g} Bx \qquad \text{(A-58)}$$

where

Krpon = hydrolysis rate of refractory particulate nitrogen (day^{-1})
Krn = minimum hydrolysis rate (day^{-1})
Krnalg = constant that relates hydrolysis to algal biomass (m^3 g^{-1} C day^{-1})

An exponential function relates mineralization and hydrolysis rates to temperature.

Nitrification

Nitrification is a process mediated by specialized groups of autotrophic bacteria that obtain energy through the oxidation of ammonium to nitrite and oxidation of nitrite to nitrate. A simplified expression for complete nitrification (Tchobanoglous and Schroeder 1987) is:

$$NH_4^+ + 2\,O_2 \rightarrow NO_3^- + H_2O + 2\,H^+ \qquad \text{(A-59)}$$

The equation indicates that two moles of oxygen are required to nitrify one mole of ammonium into nitrate. However, the simplified equation is not strictly true. Cell synthesis by nitrifying bacteria is accomplished by the fixation of carbon dioxide so that less than two moles of oxygen are consumed per mole ammonium utilized (Wezernak and Gannon 1968).

The kinetics of complete nitrification are modeled as a function of available ammonium, dissolved oxygen, and temperature:

$$NT = \frac{DO}{KHont + DO}\,\frac{NH_4}{KHnnt + NH_4}\,f(T)\,NTm \qquad \text{(A-60)}$$

where

NT = nitrification rate (g N m^{-3} day^{-1})
KHont = half-saturation constant of dissolved oxygen required for nitrification (g O_2 m^{-3})
KHnnt = half-saturation constant of NH_4 required for nitrification (g N m^{-3})
NTm = maximum nitrification rate at optimal temperature (g N m^{-3} day^{-1})

The kinetics formulation incorporates the products of two Monod functions. The first function diminishes nitrification at low dissolved oxygen concentration. The second function expresses the influence of ammonium concentration on nitrification. When ammonium concentration is low, relative to KHnnt, nitrification is proportional to ammonium concentration. For NH4 $<<$ KHnnt, the reaction is approximately first-order. (The first-order decay constant $\approx$ NTm/KHnnt.) When ammonium concentration is large relative to KHnnt, nitrification approaches a maximum rate. This formulation is based on a concept proposed by Tuffey et al. (1974). Nitrifying bacteria adhere to benthic or suspended sediments. When ammonium is scarce, vacant surfaces suitable for nitrifying bacteria exist. As ammonium concentration increases, bacterial biomass increases, vacant surfaces are occupied, and the rate of nitrification increases. The bacterial population attains maximum density when all surfaces suitable for bacteria are occupied. At this point, nitrification proceeds at a maximum rate independent of additional increase in ammonium concentration.

The optimal temperature for nitrification may be less than peak temperatures that occur in coastal waters. To allow for a decrease in nitrification at superoptimal temperature, the effect of temperature on nitrification is modeled in the Gaussian form of Equation A-14.

Effect of Nitrification on Ammonium

$$\frac{\delta}{\delta t} NH_4 = - NT \qquad \text{(A-61)}$$

Effect of Nitrification on Nitrate

$$\frac{\delta}{\delta t} NO_3 = NT \qquad \text{(A-62)}$$

Effect of Nitrification on Dissolved Oxygen

$$\frac{\delta}{\delta t} DO = - AONT\, NT \qquad \text{(A-63)}$$

where

AONT = mass dissolved oxygen consumed per mass ammonium-nitrogen nitrified (4.33 g O_2 g^{-1} N)

Effect of Denitrification on Nitrate

The effect of denitrification on dissolved organic carbon has been described. Denitrification removes nitrate from the system in stoichiometric proportion to carbon removal as determined by Equation A-39:

$$\frac{\delta}{\delta t} NO_3 = - ANDC\, Denit\, DOC \qquad \text{(A-64)}$$

where

ANDC = mass nitrate-nitrogen reduced per mass dissolved organic carbon oxidized (0.933 g N g^{-1} °C)

Nitrogen Mass Balance Equations

The mass-balance equations for nitrogen state variables are written by summing all previously-described sources and sinks:

Ammonium

$$\frac{\delta}{\delta t} NH_4 = \sum_{x=c,d,g} (BMx\ FNIx + PRx\ FNIP - PNx\ Px)\ ANCx\ Bx + Kdon\ DON - NT \quad \text{(A-65)}$$

Dissolved Organic Nitrogen

$$\frac{\delta}{\delta t} DON = \sum_{x=c,d,g} (BMx\ FNDx + PRx\ FNDP)\ ANCx\ Bx + Klpon\ LPON + Krpon\ RPON - Kdon\ DON \quad \text{(A-66)}$$

Labile Particulate Organic Nitrogen

$$\frac{\delta}{\delta t} LPON = \sum_{x=c,d,g} (BMx\ FNLx + PRx\ FNLP)\ ANCx\ Bx - Klpon\ LPON - WSl \frac{\delta}{\delta z} LPON \quad \text{(A-67)}$$

Refractory Particulate Organic Nitrogen

$$\frac{\delta}{\delta t} RPON = \sum_{x=c,d,g} (BMx\ FNRx + PRx\ FNRP)\ ANCx\ Bx - Krpon\ RPON - WSr \frac{\delta}{\delta z} RPON \quad \text{(A-68)}$$

Nitrate

$$\frac{\delta}{\delta t} NO_3 = \sum_{x=c,d,g} (PNx - 1)\ Px\ ANCx\ Bx + NT - ANDC\ Denit\ DOC \quad \text{(A-69)}$$

Silica

The model incorporates two siliceous state variables, available silica and particulate biogenic silica. For practical purposes, available silica is equivalent to dissolved silica although sorption of available silica to inorganic solids occurs. The silica cycle is a simple one in which diatoms take up available silica and recycle available and particulate biogenic silica through the actions of metabolism and predation. Particulate silica dissolves in the water column or settles to the bottom. A portion of the settled particulate biogenic dissolves within the sediments and returns to the water column as available silica. Sources and sinks represented are:

Diatom production and metabolism
Predation
Dissolution of particulate to dissolved silica
Settling
Exchange with inorganic solids

Available Silica

Dissolved silica sorb to newly-formed metal particles and rapidly settled to the bottom. To represent this process, available silica is partitioned into dissolved and particulate fractions according to a linear sorption isotherm:

$$SAd = \frac{1}{1 + Kadsa\ TAMp} SA \qquad \text{(A-70)}$$

$$SAp = \frac{Kadsa\ TAMp}{1 + Kadsa\ TAMp} SA \qquad \text{(A-71)}$$

where

SA = available silica concentration (g Si $m^{-3)}$
SAd = dissolved available silica (g Si m^{-3})
SAp = particulate available silica (g Si m^{-3})
Kadsa = partition coefficient of sorbed vs. dissolved available silica (m^3 mol^{-1})

The kinetic equation for available silica is:

$$\frac{\delta}{\delta t} SA = (FSAP\ PRd - Pd)\ ASCd\ Bd - WSs \frac{\delta}{\delta z} SAp + Ksua\ SU \qquad (A\text{-}72)$$

where

SU = particulate biogenic silica concentration (g Si m^{-3})
FSAP = fraction of diatom silica made available by predation ($0 \leq FSAP \leq 1$)
ASCd = silica-to-carbon ratio of diatoms (g Si g^{-1} C)
Ksua = particulate silica dissolution rate (day^{-1})

Particulate Biogenic Silica

The kinetic equation for particulate biogenic silica is:

$$\frac{\delta}{\delta t} SU = (BMd + (1 - FSAP)\ PRd)\ ASCd\ Bd - WSs \frac{\delta}{\delta z} SU - KSUA\ SU \qquad (A\text{-}73)$$

An exponential function describes the effect of temperature on silica dissolution.

Chemical Oxygen Demand

In the model, chemical oxygen demand is the concentration of reduced substances that are oxidizable through inorganic means. The source of chemical oxygen demand in saline water is sulfide released from sediments. A cycle occurs in which sulfate is reduced to sulfide in the sediments and reoxidized to sulfate in the water column. In freshwater, methane is released to the water column by the sediment model. Both sulfide and methane are quantified in units of oxygen demand and are treated with the same kinetic formulation:

$$\frac{\delta}{\delta t} COD = - \frac{DO}{KHocod + DO} Kcod\ COD \qquad (A\text{-}74)$$

where

COD = chemical oxygen demand concentration (g O2-equivalents m^{-3})
KHocod = half-saturation concentration of dissolved oxygen required for exertion of chemical oxygen demand (g O_2 m^{-3})
Kcod = oxidation rate of chemical oxygen demand (day^{-1})

An exponential function describes the effect of temperature on exertion of chemical oxygen demand.

Dissolved Oxygen

Sources and sinks of dissolved oxygen in the water column include:

Algal photosynthesis
Atmospheric reaeration
Algal respiration
Heterotrophic respiration
Nitrification
Chemical oxygen demand

Reaeration

The rate of reaeration is proportional to the dissolved oxygen deficit in model segments that form the air-water interface:

$$\frac{\delta}{\delta t} DO = \frac{Kr}{\Delta z} (DOs - DO) \qquad \text{(A-75)}$$

where

Kr = reaeration coefficient (m day^{-1})
DOs = dissolved oxygen saturation concentration (g O_2 m^{-3})

The surface renewal concept, attributed to Danckwerts by O'Connor and Dobbins (1958), indicates:

$$Kr = \sqrt{Dl\, R} \qquad \text{(A-76)}$$

where

Dl = molecular diffusivity of oxygen in water (≈ 1.7 x 10-4 m^2 day^{-2})
R = surface renewal rate (day^{-1})

Specification of the surface renewal rate is the fundamental problem in reaeration theory. O'Connor and Dobbins (1958) state that, in isotropic turbulence, surface renewal can be approximated as the ratio of stream velocity to depth. The renewal rate is also influenced by wind (O'Connor 1983). Influences of temperature (ASCE 1961) and salinity (Wen et al. 1984) on aeration, most likely effected through changes in diffusivity, have been measured. No single theory that unites all these factors into a formulation of reaeration in an estuary is available. The surface renewal concept is retained with the renewal rate treated as a calibration parameter.

Saturation dissolved oxygen concentrations decrease as temperature and salinity increase. An empirical formula that describes these effects (Genet et al. 1974) is:

$$DOs = 14.5532 - 0.38217\,T + 0.0054258\,T^2 - (1.665 \times 10^{-4} - 5.866 \times 10^{-6}\,T + 9.796 \times 10^{-8}\,T^2)\,CL \quad \text{(A-77)}$$

where

CL = chloride concentration (= salinity/1.80655)

Summary of Dissolved Oxygen Sources and Sinks

The complete kinetics for dissolved oxygen are:

$$\frac{\delta}{\delta t} DO = \sum_{x=c,d,g} \left[(1.3 - 0.3\,PNx)\,Px - \frac{DO}{KHrx + DO} BMx \right] AOCR\,Bx - AONT\,NT - \frac{DO}{KHodoc + DO} AOCR\,Kdoc\,DOC - \frac{DO}{KHocod + DO} Kcod\,COD + \frac{Kr}{\Delta z}(DOs - DO) \quad \text{(A-78)}$$

Total Active Metal

The total active metal state variable is the sum of iron and manganese concentrations. Iron and manganese exist in particulate and dissolved forms in estuaries. The prime determinant of the species is dissolved oxygen. In the oxygenated water, total iron and manganese are almost completely particulate. Under anoxic conditions, large fractions of total iron and manganese are dissolved although solid-phase sulfides and carbonates exist and may predominate. The simplified partitioning of particulate and dissolved phases of total active metal employed here notes that total active metal concentration must achieve a minimum level before precipitation occurs. The minimum level is a function of dissolved oxygen:

$$TAMd = \text{minimum}\,(TAMdmx\,e^{-Kdotam\,DO}, TAM) \quad \text{(A-79)}$$

$$TAMp = TAM - TAMd \quad \text{(A-80)}$$

where

TAM = total active metal concentration (mol m^{-3})
TAMd = dissolved total active metal (mol m^{-3})
TAMp = particulate total active metal (mol m^{-3})

TAMdmx = solubility of total active metal under anoxic conditions (mol m^{-3})
Kdotam = constant that relates total active metal solubility to dissolved oxygen concentration (m^3 g^{-1} O_2)

The origin of total active metal in the model is benthic sediments. Since metal release is not explicit in the sediment model, release is incorporated into the kinetics portion of the water-column model. Release is treated as a spatially-uniform, empirical function of temperature and dissolved oxygen concentration. The only other source or sink in the water column is settling of the particulate fraction. In the mass balance equation, the benthic source operates only in model cells that adjoin the bottom:

$$\frac{\delta}{\delta t} TAM = - WSs \frac{\delta}{\delta z} TAMp + \frac{KHbmf}{KHbmf + DO} \frac{BENTAM}{\Delta z} \qquad (A\text{-}81)$$

where

BENTAM = anoxic total active metal release rate release rate (mol m^{-2} day^{-1})
KHbmf = dissolved oxygen concentration at which total active metal release is half the anoxic rate (g O_2 m^{-3})

Release of metal from the bottom is maximum when dissolved oxgyen is absent from the overlying water. Release declines as oxygen concentration increases and is negligible when dissolved oxygen $>>$ KHbmf.

Sediment release of total active metal is treated as an exponential function of temperature.

Salinity

No internal sources or sinks of salinity exist.

Temperature

The only source or sink of internal energy considered is exchange with the atmosphere. Although solar radiation can penetrate several meters into the water column, radiation-induced increases in internal energy are assigned entirely to the surface model layer.

The internal-energy equation can be written as a conservation of temperature equation. Change in temperature due to atmospheric exchange is considered proportional to the temperature difference between the water surface and a theoretical equilibrium temperature (Edinger et al. 1965):

$$\frac{\delta}{\delta t} T = \frac{KT}{\rho \, Cp \, \Delta z} (Te - T) \qquad \text{(A-82)}$$

where

Te = equilibrium temperature (°C)
KT = Heat exchange coefficient (W m^{-2} °C^{-1})
Cp = specific heat of water (4200 W sec kg^{-1} °C^{-1})
ρ = density of water (1000 kg m^{-3})