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DERIVATION OF A THREE DIMENSIONAL NUMERICAL WATER QUALITY MODEL FOR ESTUARY AND CONTINENTAL SHELF APPLICATION

By Malcolm Spaulding

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DERIVATION OF A THREE DIMENSIONAL NUMERICAL WATER QUALITY MODEL FOR ESTUARY AND CONTINENTAL SHELF APPLICATION

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SUMMARY

A derivation is given for a three dimensional mass transport equation which is appropriate for numerical modeling of estuary and Continental Shelf water quality variations for both the time dependent and steady state cases. A stable and accurate finite difference approximation to the derived equation is presented and a solution scheme for the resulting equations outlined. Preliminary results are obtained using the model for extremely simple problems which have analytical solutions. The results indicate that the numerical model as presented will provide a fruitful scheme to study water quality problems in coastal waters for both steady state and time dependent cases.

INTRODUCTION

The ability to quantitatively assess the influence of waste discharges on the water quality of receiving waters to ensure their proper management has progressed rather rapidly in recent years. Development of mathematical or numerical water quality models for the one dimensional (1,2,3,4) and two dimensional (5,6,7,8,9,10) cases have been shown to provide a basis for prediction of various water disposal alternatives and their effect on water quality. Summaries of the status of research in this area are provided in state-of-the-art reports cited in References (11) and (12).

In each of these models, however, an assumption has been made that one or several of the spatial dimensions is not significant for the particular area under study. For instance, the one-dimensional approximations normally assume that the vertical and cross stream structure of a given water quality parameter is of secondary importance while the longitudinal or main axis of flow directions is of primary interest. Two-dimensional models characteristically eliminate either the vertical or lateral structure while maintaining the other two. This integral or averaging approach has normally been taken, since as the number of spatial dimensions increases, the computational difficulties, as well as computer time and storage requirements to solve the

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resulting equations, increases markedly. There are, however, regions both in estuaries and on the Continental Shelf, where a useful representation of the actual water quality distribution can only be obtained from a three-dimensional picture.

In addition to averaging over the spatial dimensions to eliminate spatial fluctuations of water quality indicators, it is also possible to average the predictions over some time scale, ranging from the order of a portion of a tidal cycle to many days. These models then, generally are classified as time-dependent and steady-state, respectively, and each provide an important approach to coastal zone pollution studies.

The present work will derive a three-dimensional mass transport equation appropriate for numerical modeling of estuaries and Continental Shelf water quality variations for both the time-dependent and steady-state cases. A finite difference approximation to the original equation will be shown and a solution scheme for the resulting equations outlined. The tidal hydraulics or coastal circulation is assumed to be known from field data or hydraulic model studies.

SYMBOLS

C	coliform bacteria concentration
C_S	source of coliform bacteria
C_z	Chezy coefficient
D_x, D_y, D_z	dispersion coefficient in x, y, and z directions respectively
D	mean sea level depth
e_x, e_y, e_z	turbulent diffusion coefficients in x, y, and z directions respectively
g	gravity acceleration
H	total depth, mean sea level depth plus tidal height
J	discharge rate of B.O.D.
K_A	reaeration coefficient for D.O.
K_d	decay coefficient for coliform bacteria
K_L	B.O.D. decay coefficient
L	biological oxygen demand (B.O.D.) concentration

O	dissolved oxygen (D.O.) concentration
O_{SAT}	D.O. saturation level
$\vec{P}$	mass density or concentration vector
R_i	Richardson number
S	salinity or source (sink) strength
S_o	source (sink) strength of D.O.
$\vec{S}$	source (sink) vector
t	time
$\bar{u}$,U	mean flow speed
u,v,w	velocities components in x, y, and z direction respectively
WH	wave height
WL	wave length
WT	wave period
x,y,z	rectangular cartesian coordinates

Greek symbols

$\alpha_p, \beta_p, \eta_p$	empirical constants for equation 2.11
$\delta_x, \delta_y, \delta_\eta$	difference operators defined by equation 3.3
η	nondimensional height coordinate
ω	nondimensional vertical velocity
ρ_A	mass density or concentration of substance A
ξ	tidal height

MASS TRANSPORT MODEL

Derivation of Mass Transport Equation

To accurately predict the movement of a water quality parameter, requires one to quantitatively answer

(a) How is a given pollutant from a source transported and distributed through the receiving water as a function of time?

(b) How rapidly does the decay or generation by natural processes add or subtract from the water quality parameter being employed as an indicator?

The first question is primarily one involving the fluid mechanics of mass transport. The processes involved are advective transport of a constituent due to the mean tidal velocity and dispersive transport produced by turbulent mixing. These variables are related to physical hydrodynamic characteristics of the area under consideration and are both time and space dependent. The second question is chiefly concerned with chemical and microbiological processes of species generation and decay which are temperature, time, and concentration dependent. The conceptual separation employed here will be more clearly illustrated for specific water quality variables later in this report.

From these elementary considerations, numerical water quality models describing both the hydrodynamic transport and decay or generation of a specific constituent assume the form of a mass transport equation with a specific set of source-sink or reaction matrix terms. The exact form of the reaction matrix, as shown in the next section, depends on whether the constituent is conservative or nonconservative and whether its magnitude depends on other constituent concentrations. Examples of this conceptual approach are presented in references (6) and (10).

In the following paragraphs, the basic mass transport equation will be presented and in a later section it will be shown how this can be extended to include water quality parameters.

In a turbulent medium the mass transport equation for a given constituent may be written (13, 14) as:

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial \rho_A u}{\partial x} + \frac{\partial \rho_A v}{\partial y} + \frac{\partial \rho_A w}{\partial z} = \frac{\partial}{\partial x}\left(e_x \frac{\partial \rho_A}{\partial x}\right) + \frac{\partial}{\partial y}\left(e_y \frac{\partial \rho_A}{\partial y}\right) + \frac{\partial}{\partial z}\left(e_z \frac{\partial \rho_A}{\partial z}\right) + S \quad (2.1)$$

where

ρ_A - mass density or concentration of substance A

e_x, e_y, and e_z - turbulent diffusion coefficients

u, v, and w - time mean velocity over short sampling times in the x, y, and z directions respectively

S - source or sink of substance A

In this form, several approximations have already been introduced. Molecular diffusion has been neglected in anticipation that in the environments under consideration it is several orders of magnitude smaller than the turbulent eddy diffusivity. The diffusion terms are obtained by assuming that the turbulent flux terms such as $u'\rho_A'$ can be adequately modeled by the product of an eddy diffusion coefficient and the ensemble mean concentration gradient. It has also been assumed that no diffusive transports are caused by thermal or pressure gradients within the system. The velocities in the system represent time averages over short sampling periods much smaller than a tidal cycle but larger than the instantaneous variations i.e. one minute periods. This procedure then eliminates the stochastic variations in mass density. The approximations that have been shown are essentially valid for estuary and Continental Shelf waters (14, 15).

A coordinate system (fig. 1) can be chosen with z measured vertically upward from the bottom or x and y plane where x is the longitudinal axis and y is the lateral axis. The water level caused by the ebb and flood of the tide, then is a perturbation, ξ, above or below the mean sea level plane.

In order to make the mass transport equation more adaptable to the large scale depth variations found in estuary and Continental Shelf regions, and also to eliminate troublesome numerical boundary conditions at the sea bed and free surface it has been found convenient to nondimensionalize the vertical axis using the total depth, that is mean sea level depth plus instantaneous tidal height. The resulting mass transport equation then becomes:

$$\frac{\partial(H\,\rho_A)}{\partial t} + \frac{\partial(H\,u\rho_A)}{\partial x} + \frac{\partial(H\,v\rho_A)}{\partial y} + \frac{\partial(H\,\omega\rho_A)}{\partial \eta}$$

$$= \frac{\partial}{\partial x}\left(He_x \frac{\partial \rho_A}{\partial x}\right) + \frac{\partial}{\partial y}\left(He_y \frac{\partial \rho_A}{\partial y}\right) + \frac{\partial}{\partial \eta}\left(\frac{e_z}{H} \frac{\partial \rho_A}{\partial \eta}\right) + SH \qquad (2.2)$$

where $\frac{\partial H}{\partial x}$ and $\frac{\partial H}{\partial y}$ have been assumed small and

H - total depth, mean sea level depth plus tidal height $(D + \xi)$

D - mean sea level depth

ξ - tidal height

$\eta = z/H$

and the relationship between the real vertical velocity, w, and the nondimensional vertical velocity, ω, is given by:

$$w = \eta\left(\frac{\partial H}{\partial t} + u \frac{\partial H}{\partial x} + v \frac{\partial H}{\partial y}\right) + \omega H \qquad (2.3)$$

where the derivatives are evaluated holding η constant.

Equation (2.2) then represents a mathematical model for the convection and dispersion of any constituent ρ_A with a generalized source or sink combination of strength S.

Reaction Model

Water quality models, as previously stated, generally assume the form of a mass transport equation as shown in eq. (2.2) with a specific source--sink or reaction matrix term which has been simply noted as S. In the present section, the details of this reaction matrix term will be presented for several water quality parameters.

To aid in the discussion, it is noted that water quality parameters can be divided into two general classes--conservative and nonconservative models. The non-conservative models can be further subdivided into those containing multistage reaction schemes. In order to better understand this division, a few examples are presented.

1. Conservative Case (Salinity)

$$\frac{\partial S}{\partial t} + \frac{\partial uS}{\partial x} + \frac{\partial vS}{\partial y} + \frac{\partial wS}{\partial z} - \frac{\partial}{\partial x}\left(e_x \frac{\partial S}{\partial x}\right) - \frac{\partial}{\partial y}\left(e_y \frac{\partial S}{\partial y}\right) - \frac{\partial}{\partial z}\left(e_z \frac{\partial S}{\partial z}\right) = 0$$

S - salinity or chlorinity (2.4)

2. Nonconservative, Single-Stage Reaction Case (Coliform)

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} + \frac{\partial wC}{\partial z} - \frac{\partial}{\partial x}\left(e_x \frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial y}\left(e_y \frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial z}\left(e_z \frac{\partial C}{\partial z}\right) = K_d C + C_S \quad (2.5)$$

C - coliform bacteria concentration

K_d - decay rate for coliform bacteria

C_S - source of coliform bacteria

3. Nonconservative, Two-Stage Reaction Case

(Dissolved Oxygen (D.O) and Biochemical Oxygen Demand (B.O.D.)

$$\frac{\partial L}{\partial t} + \frac{\partial uL}{\partial x} + \frac{\partial vL}{\partial y} + \frac{\partial wL}{\partial z} - \frac{\partial}{\partial x}\left(e_x \frac{\partial L}{\partial x}\right) - \frac{\partial}{\partial y}\left(e_y \frac{\partial L}{\partial y}\right) - \frac{\partial}{\partial z}\left(e_z \frac{\partial L}{\partial z}\right) =$$

$$- K_L L + J(x,y,z,t) \tag{2.6}$$

$$\frac{\partial O}{\partial t} + \frac{\partial uO}{\partial x} + \frac{\partial vO}{\partial y} + \frac{\partial wO}{\partial z} - \frac{\partial}{\partial x}\left(e_x \frac{\partial O}{\partial x}\right) - \frac{\partial}{\partial y}\left(e_y \frac{\partial O}{\partial y}\right) - \frac{\partial}{\partial z}\left(e_z \frac{\partial O}{\partial z}\right) =$$

$$- K_L L + K_A(O_{SAT} - O) - S_O \tag{2.7}$$

L - B.O.D. concentration

O - D.O. concentration

K_L - B.O.D. decay coefficient

J - point load of B.O.D. due to outfall

K_A - reaeration coefficient for D.O.

O_{SAT} - D.O. saturation level

S_O - source or sink of D.O.

From these elementary examples, one can see the essential mass transport equation on the left-hand side of the equal sign remaining unchanged in form, and the varying source-sink terms on the right-hand side.

In an attempt to generalize Eq. (2.2) for all water quality parameters, we can assume that S, the source-sink term, can be subdivided as:

$$S = [K]\vec{P} + \vec{S}$$

where $\vec{S}$ - source or sink vector

$[K]$ - reaction matrix

$\vec{P}$ - mass density or concentration vector

then eq. (2.2) may be expressed as

$$\frac{\partial \vec{P}}{\partial t} + \frac{\partial u\vec{P}}{\partial x} + \frac{\partial v\vec{P}}{\partial y} + \frac{\partial w\vec{P}}{\partial z} - \frac{\partial}{\partial x}\left(e_x \frac{\partial \vec{P}}{\partial x}\right) - \frac{\partial}{\partial y}\left(e_y \frac{\partial \vec{P}}{\partial y}\right) - \frac{\partial}{\partial z}\left(e_z \frac{\partial \vec{P}}{\partial z}\right) = [K]\vec{P} + \vec{S} \tag{2.8}$$

This provides a general equation for all water quality parameters or reaction schemes. In its most general form, this approach allows for decay or birth rates dependent on concentration levels of any individual or group of constituents, as well as multistage reaction mechanisms.

As a simple illustration of how this generalization encompasses the previous examples, let us look at the reaction matrix for salinity.

$$\vec{P} = [P_1] \quad \text{where} \quad P_1 \text{ - salinity}$$

$$K = [0]$$

$$\vec{S} = [0]$$

and for the multistage D.O. - B.O.D. system

$$\vec{P} = \begin{bmatrix} P_1 \\ P_2 \end{bmatrix} \quad \begin{matrix} P_1 \text{ - D.O. concentration} \\ P_2 \text{ - B.O.D. concentration} \end{matrix}$$

$$K = \begin{bmatrix} -K_A & -K_L \\ 0 & -K_L \end{bmatrix}$$

$$\vec{S} = \begin{bmatrix} K_A O_{SAT} + S_O \\ J \end{bmatrix}$$

where the variables have been previously defined. Pulse loads of waste B.O.D. defined by J are handled as pulse loads to the sink-source vector $\vec{S}$ at appropriate spatial locations.

The generalization of all water quality equations to this conceptual form provides a simplification of numerical models since it provides a relatively easily handled programming technique to deal with a great variety of water quality problems.

Dispersion in Multi-dimensional Computations

In our derivation of the mass transport equation, it was assumed that the normal turbulent mass transport terms such as $u'\rho_A'$ could be adequately represented by a diffusion coefficient times the mean concentration gradient. It then remains to determine either analytical or empirical expressions that can be employed to represent these terms.

In anticipation of using a finite difference approach for the solution of our mass transport equation for which a finite or discrete space is assumed to have fixed properties, we must ask ourselves how this approach could effect any estimates that are made for the diffusion coefficient in question. Physically the discretization process averages the velocities, mass densities, and any other variables over the region of our finite space increments. Therefore, in any formulation that is made for diffusion coefficients we must remember this averaging process has been performed.

The work of Fischer (16) provides a straightforward explanation of the mechanisms involved in the diffusion of constituents in real environments and will provide the basis for determining the coefficients in light of the finite difference approximation. In general, various parts of natural water environments taken perpendicular to the mean flow show differences in velocity. Due to these variations, portions of a field of pollutant constituent will move more or less rapidly than the mean flow, hence dispersing the pollutant in the direction of the flow. This process then causes cross sectional variations in the mass concentration and leads to a cross sectional turbulent diffusion which tends to transfer constituents from parts with higher concentration to those with lower concentration. This explanation is valid for the contributions from both the vertical and lateral variations in the mean flow. Reviewing this description,we have included not only the turbulent diffusion but also the effect of shear in the velocity profiles if a finite approximation for a spatial grid is used. Under these circumstances the "diffusion" coefficients are called dispersion coefficients and will be noted in the remainder of this report by D_x, D_y, and D_z for the x, y, and z coordinate directions.

Elder (17) based on Taylor's (18) concept has determined expressions for the longitudinal and lateral dispersion coefficients based on the mean velocity, depth, and bottom roughness for simple one-dimensional steady flow which should be useful in our problem. Their expressions are:

$$D_x = 5.93\, D\bar{u}\, g^{1/2}\, C_z^{-1} \tag{2.9}$$

and

$$D_y = .23\, D\bar{u}\, g^{1/2}\, C_z^{-1} \tag{2.10}$$

where

$\bar{u}$ - mean uniform flow speed

g - gravitational acceleration

C_z - Chezy coefficient

D - water depth

Expressions of this type, with a correction of an additive constant for wind effects, have been used rather successfully by Leenderste (7) in two-dimensional, vertically-averaged, water quality modeling and should provide reasonable results in the present work.

Using an approach based on work by Pritchard et al. (19, 20, 21) in the James River estuary, an approximate form of a vertical dispersion coefficient--founded on a mixing length theory--which includes both stratification and surface mixing due to the wind has been proposed. The formulation is given as:

$$D_z = \eta_P \frac{U_z^2 (D - Z)^2}{D^3} (1 + \beta_P R_i)^{-2} + \alpha_P \frac{Z(D - Z)}{D} \frac{WH}{WT} e^{-\frac{2\pi Z}{WL}}$$

$$x (1 + \beta_P R_i)^{-2} \qquad (2.11)$$

where

$\eta_P, \beta_P, \alpha_P$ adjustable coefficients dependent on particular region of interest

U - mean flow speed

D - mean sea level depth

Z - distance measured vertically downward from mean sea level

R_i - Richardson number $[g/\rho \; \partial\rho/\partial Z/(.7 \frac{\bar{u}}{D})^2]$

WH - wave height

WL - wave length

WT - wave period

Although this formulation has only been shown to be strictly applicable to the James River area under essentially steady-state conditions, it provides a good first estimate and could--through the variable constants--probably be adapted to give reasonable results for our area of concern.

As presented, the values of dispersion obtained from various works in the literature show that if a comparison of vertical to longitudinal or lateral dispersion coefficients is made the former is always several orders of magnitude smaller than the latter two. This fact complicates the modeling effort since dispersion becomes anisotropic. However, using arguments from the work of Holley (22), it can be shown that for most coastal marine environments the movement or transport of a particular constituent is determined largely by the advection rather than dispersive transport process in the mean sea level plane, and, hence, lateral or longitudinal dispersion is a secondary effect. (This is not true in areas immediately surrounding an outfall.) Therefore, one can assume an isotropic approximation in each direction, and ignore anisotropic effects.

As a general approach, one finds that as the ability to accurately predict the three-dimensional time dependent velocity field increases the importance of the dispersion terms decreases. Hence for any particular model development, tests should be performed to ascertain the sensitivity to changes in dispersion coefficient. This will be mainly dependent on how accurate--the size of spatial grids and type of averaging of the tidal hydraulic equations--the velocity or circulation is determined. Therefore, the more accurate the circulation picture is known, the less we need to be concerned with the dispersive transport mechanism.

COMPUTATIONAL MODEL

Derivation of Finite Difference Approximation

Time-Dependent Model.- The mass transport equation as developed in equation (2.2) permits a rather large number of finite difference approximations. For each possible approach, an analysis of the convergence and stability characteristics has to be performed such that assurance is gained that the difference approximations will actually represent the solution to the proposed equation. Following earlier computational work in the field of mass transport modeling, notably the work of Leenderste, (6), an extension of the A.D.I. (Alternating Direction Implicit) technique was considered as the most versatile of the methods since it has unconditional stability but only tridiagonal equations to be solved for each direction in space.

The computational model presented here for the mass transport equation is based on the methods developed by Douglas (23), Douglas and Gunn (24) and others (25, 26).

As a first step, a space staggered grid system is chosen to locate the discrete values of the variables. (fig. 2.) It is to be noted that this

choice of grid formulation provides centrally-located spatial derivatives for the linear terms. In addition, the mass density previously defined as ρ_A which is a point function will be replaced by P indicating that an averaging over a physical volume corresponding to the spatial grid size has occurred. The following notation for defining discrete values for the finite difference approximations will be used.

$$\begin{aligned} x &= m\,\Delta x \\ y &= k\,\Delta y \\ \eta &= n\,\Delta\eta \\ t &= \ell\,\Delta t \end{aligned} \tag{3.1}$$

where m,k,n,ℓ - integers

$\Delta x,\Delta y,\Delta\eta$ - spatial grid sizes in the x, y, and η coordinate directions

Δt - temporal

Therefore, the mass density of a given constituent can be expressed in finite difference form as:

$$P(x,y,\eta,t) = P(m\Delta x,k\Delta y,n\Delta\eta,\ell\Delta t) = P^{\ell}_{m,k,n} \tag{3.2}$$

and also defining the difference operators as:

$$\begin{aligned} \delta_x P^{\ell}_{m,k,n} &= P^{\ell}_{m+1/2,k,n} - P^{\ell}_{m-1/2,k,n} \\ \delta_y P^{\ell}_{m,k,n} &= P^{\ell}_{m,k+1/2,n} - P^{\ell}_{m,k-1/2,n} \\ \delta_\eta P^{\ell}_{m,k,n} &= P^{\ell}_{m,k,n+1/2} - P^{\ell}_{m,k,n-1/2} \end{aligned} \tag{3.3}$$

Now employing the approach which Douglas (23) originally used on the heat conduction problem, equation (2.2) can be approximated in finite difference form by the three following equations:

$$- \frac{1}{2}\delta_x(UHP)^{\ell+1/3} - \frac{1}{2}\delta_x(UHP)^{\ell} + \frac{1}{2}\delta_x(D_xH\delta_x(P))^{\ell+1/3}$$

$$+ \frac{1}{2}\delta_x(D_xH\delta_x(P))^{\ell} - \delta_y(VHP)^{\ell} - \delta_\eta(\omega HP)^{\ell} + \delta_y(D_yH\delta_y(P))^{\ell}$$

$$- \delta_\eta\left(\frac{D_z}{H}\delta_\eta(P)\right)^{\ell} + (SH)^{\ell} = \frac{(HP)^{\ell+1/3} - (HP)^{\ell}}{\Delta t} \tag{3.4}$$

advancing the solution from time level ℓ to time level $\ell + 1/3$ and

$$- \frac{1}{2}\delta_x(UHP)^{\ell+1/3} - \frac{1}{2}\delta_x(UHP)^{\ell} + \frac{1}{2}\delta_x(D_xH\delta_x(P))^{\ell+1/3}$$

$$+ \frac{1}{2}\delta_x(D_xH\delta_x(P))^{\ell} - \frac{1}{2}\delta_y(VHP)^{\ell+2/3} - \frac{1}{2}\delta_y(VHP)^{\ell}$$

$$+ \frac{1}{2}\delta_y(D_yH\delta_y(P))^{\ell+2/3} + \frac{1}{2}\delta_y(D_yH\delta_y(P))^{\ell} - \delta_\eta(\omega HP)^{\ell}$$

$$+ \delta_\eta\left(\frac{D_z}{H}\delta_\eta(P)\right)^{\ell} = \frac{(HP)^{\ell+2/3} - (HP)^{\ell}}{\Delta t} \tag{3.5}$$

advancing the solution from time level $\ell + 1/3$ to time level $\ell + 2/3$ and

$$- \frac{1}{2}\delta_x(UHP)^{\ell+1/3} - \frac{1}{2}\delta_x(UHP)^{\ell} + \frac{1}{2}\delta_x(D_xH\delta_x(P))^{\ell+1/3}$$

$$+ \frac{1}{2}\delta_x(D_xH\delta_x(P))^{\ell} - \frac{1}{2}\delta_y(VHP)^{\ell+2/3} - \frac{1}{2}\delta_y(VHP)^{\ell}$$

$$+ \frac{1}{2}\delta_y(D_yH\delta_y(P))^{\ell+2/3} + \frac{1}{2}\delta_y(D_yH\delta_y(P))^{\ell}$$

$$- \frac{1}{2}\delta_\eta(\omega HP)^{\ell+1} - \frac{1}{2}\delta_\eta(\omega HP)^{\ell} + \frac{1}{2}\delta_\eta\left(\frac{D_z}{H}\delta_\eta(P)\right)^{\ell+1}$$

$$+ \frac{1}{2}\delta_\eta\left(\frac{D_z}{H}\delta_\eta(P)\right)^{\ell} = \frac{(HP)^{\ell+1} - (HP)^{\ell}}{\Delta t} \tag{3.6}$$

advancing the solution from time level $\ell + 2/3$ to time level $\ell + 1$.

An algebraic simplification of the above equations can be obtained by subtracting (3.4) from (3.5) and (3.5) from (3.6), respectively. After rearrangement the resulting equations become

$$-\delta_x(UHD)^{\ell+1/3} + \delta_x(D_x H\delta_x(P))^{\ell+1/3} - \frac{2}{\Delta t}(HP)^{\ell+1/3}$$

$$= \delta_x(UHP)^{\ell} - \delta_x(D_x H\delta_x(P))^{\ell} + 2\delta_y(VHP)^{\ell}$$

$$+ 2\delta_\eta(\omega HP)^{\ell} - 2\delta_y(D_y H\delta_y(P))^{\ell} - 2\delta_\eta\left(\frac{D_z}{H}\delta_\eta(P)\right)^{\ell}$$

$$- \frac{2}{\Delta t}(HP)^{\ell} + 2HS^{\ell+1/2} \quad . \tag{3.7}$$

$$\delta_y(D_y H\delta_y(P))^{\ell+2/3} - \delta_y(VHP)^{\ell+2/3} - \frac{2}{\Delta t}(HP)^{\ell+2/3} =$$

$$\delta_y(D_y H\delta_y(P))^{\ell} - \delta_y(VHP)^{\ell} - \frac{2}{\Delta t}(HP)^{\ell+1/3} \quad . \tag{3.8}$$

$$- \delta_\eta(\omega HP)^{\ell+1} + \delta_\eta\left(\frac{D_z}{H}\delta_\eta(P)\right)^{\ell+1} - \frac{2}{\Delta t}(HP)^{\ell+1} =$$

$$- \delta_\eta(\omega HP)^{\ell} + \delta_\eta\left(\frac{D_z}{H}\delta_\eta(P)\right)^{\ell} - \frac{2}{\Delta t}(HP)^{\ell+2/3} \tag{3.9}$$

Equations (3.7), (3.8), and (3.9) now form a finite difference approximation to the original mass transport equation of order $0((\Delta x)^2 + (\Delta t)^2)$ and can be solved for any particular rectangular grid system by solving the associated tridiagonal linear equations once for each equation. References 6 and 10 provide greater details of this approach and show how both open and closed boundaries can be handled.

Steady-State Model.- Since there are many situations when the steady-state solution of the mass transport equation (elliptic equation) is of particular interest in an area under study, it would be desirable to determine necessary modifications to the existing numerical procedure to handle this situation. Following the work of Douglas (23) and Wachpress (27) the time step increment Δt in Eqs. (3.7), (3.8) and (3.9) can be replaced by a positive number iteration parameter or sequence of iteration parameters and by iteration with these parameters a steady state solution obtained.

The problem then becomes, after convergence of the solution is assumed, the determination of a sequence of iteration parameters which when applied in some cyclic pattern will cause the rate of convergence to be maximized. Since the literature (23, 24, 27) provides only an indication of possible iteration parameters for a simple heat diffusion problem with constant dispersion, an optimum sequence of parameters is not available for the general mass transport equation and normally has to be determined through numerical experiments. Indications have been made in the work of Aziz and Hellums (28) of a possible set of iteration parameters but are not directly applicable to this case.

Extension of Numerical Model to Include Multistage Water Quality Parameters.-

Using the reaction matrix approach, as previously outlined, the computational scheme can be extended to include multistage reactions appropriate to simulate various water quality reaction systems by altering the generalized source-sink term $(HS)^{\ell+1/2}$ as noted in Equation (3.7). An appropriate numerical approximation then becomes:

$$(HS_i)^{\ell+1/2} = \sum_{j=1}^{j_{max}} (H\, K_{ij}\, P_j)^{\ell+1/2} + (HS_i)^{\ell+1/2} \qquad (3.10)$$

where

i - specific element of the mass density vector $\vec{P}$

j_{max} - maximum number of constituents

K - reaction matrix (reaction coefficients)

S_i - sources or sinks of mass density i

H - total coastal water depth

Note that P now becomes a mass concentration or density vector containing j_{max} constituents and each of these must be solved at each complete time step. Careful examination of the terms in Equation (3.10) shows that the mass density of a given constituent must be evaluated at time level $\ell + 1/2$, however when solving Equation (3.7) containing this term information for $P^{\ell+1/2}$ is not available. Douglas (23) has shown that if P is evaluated at the lower known time level ℓ, then the numerical solution has only $O((\Delta t) + (\Delta x)^2)$ accuracy. The original accuracy can be regained by estimating a value of $P^{\ell+1/2}$ by using Equations (3.7), (3.8) and (3.9) and then going back and readvancing the solution in time with the new best estimate for $P^{\ell+1/2}$. This procedure, however, essentially requires a doubling of the computational time to simulate a fixed physical time, and, therefore, should be employed with a consideration of the trade-off between computational time and accuracy.

EFFECTS OF COMPUTATIONAL MODEL APPROXIMATIONS

Stability and Convergence

Douglas (23) has shown that for the simple time dependent and steady state heat conduction equation the finite difference approximation scheme presented yields both a stable and convergent solution with an accuracy of $O((\Delta t)^2 + (\Delta x)^2)$. Indications from other work (28) also indicates that at

least in numerical experiments, these properties of convergence and stability are still valid when the lower order advection terms are included, as in the mass transport equation. Theoretical proof of this case, as far as the author knows, has not been determined at this time.

Mass Conservation

Another extremely important aspect of any numerical approach to the mass transport equation is that mass should be conserved both over the entire field under consideration as well as on the near-field or grid point scale. Preliminary results with the model as outlined show that for at least the simple case of flow in channels of variable depths that this condition is adequately met (under 1 percent cumulative mass loss or gain over several days simulation).

RESULTS

To date, the results have been only of a preliminary nature in which results for extremely simple problems have been obtained. The time dependent model has been run for simple channel cases of both constant and varying depths and has shown mass conservation within 0.1 percent over several days simulation. The case of simple dispersion--(no advection) has been performed for a typical estuary geometry with insignificant mass losses or gains. Attempts have also been made to link a two-dimensional vertically averaged tidal model to the present mass transport model, but have met with only limited success. Although the overall mass conservation appears to be within acceptable bounds, local perturbations of mass density near sharply varying geometric features cause local variations of the order of 0-4 percent of the mean field concentration.

The steady-state model has been run using a sequence of iteration parameters in a cyclic manner for a simple one-dimensional constant velocity, constant dispersion, uniform channel flow. The sequence of parameters have been chosen based on numerical experiments and is by no means the optimum, but provides reasonable convergence rates.

Figure 3 shows a comparison between the analytical and numerical solution to the simple case stated above for several combinations of velocity u, dispersion D_x, and numerical grid spacing Δx. The results were obtained by 20 cycles of the iteration sequence

$$5 \times 10^{-6}$$

$$2.5 \times 10^{-5}$$

$$1.25 \times 10^{-4}$$

$$6.25 \times 10^{-4}$$

$$3.125 \times 10^{3}$$

over a grid field (32 x 12 x 7) in 5 minutes on a CDC 6600 computer with an absolute error of 10^{-5}.

CONCLUSIONS

A derivation has been given for a three-dimensional mass transport equation which is appropriate for numerical modeling of estuary and Continental Shelf water quality variations for both the time-dependent and steady-state cases. A stable and accurate finite difference approximation to the derived equation was presented and a solution scheme for the resulting equations outlined. Preliminary results were obtained using the model for extremely simple problems which have analytical solutions. These results indicate that the numerical model, as presented, will provide a fruitful scheme to study water quality problems in coastal waters for both steady-state and time-dependent cases.

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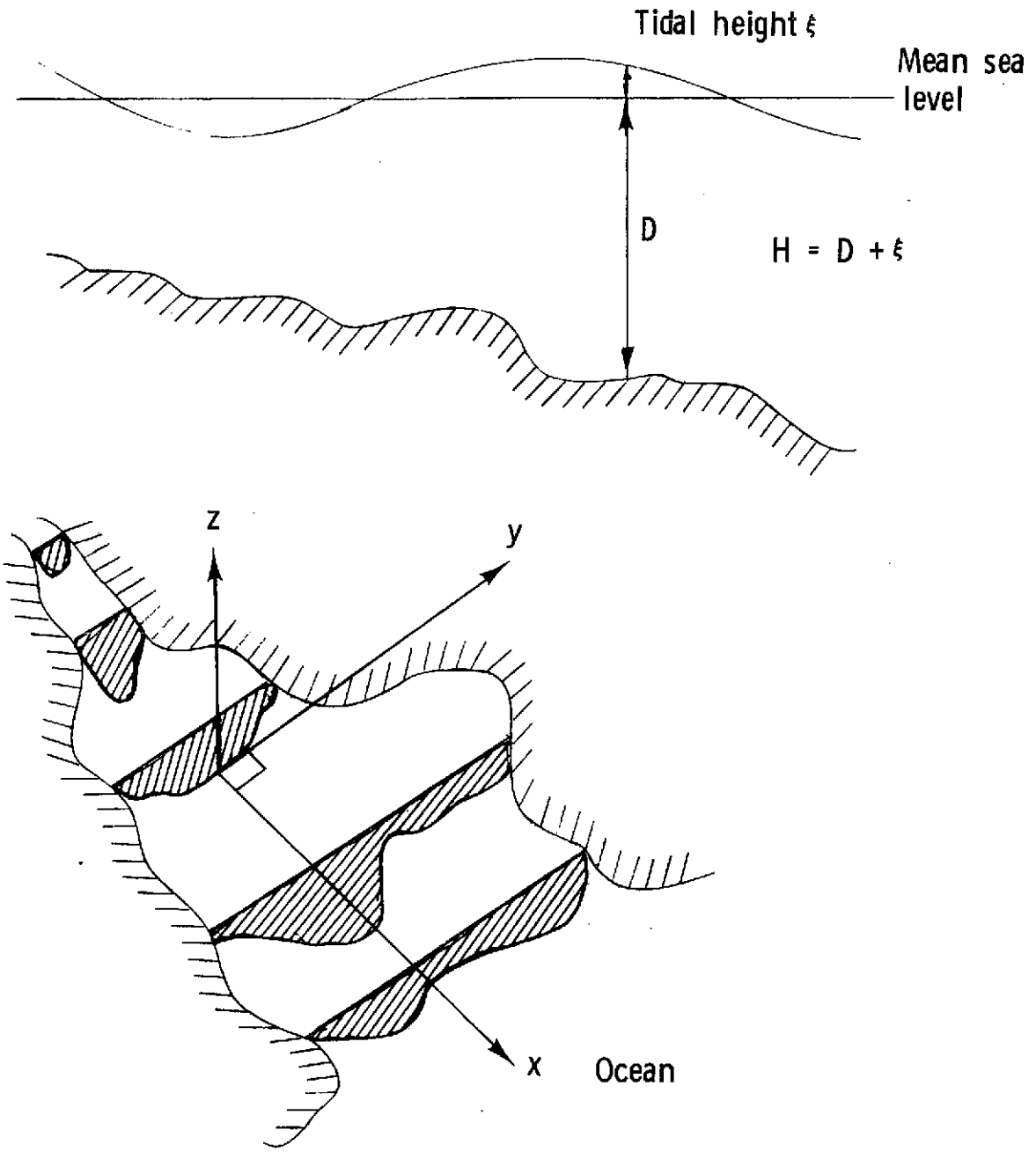
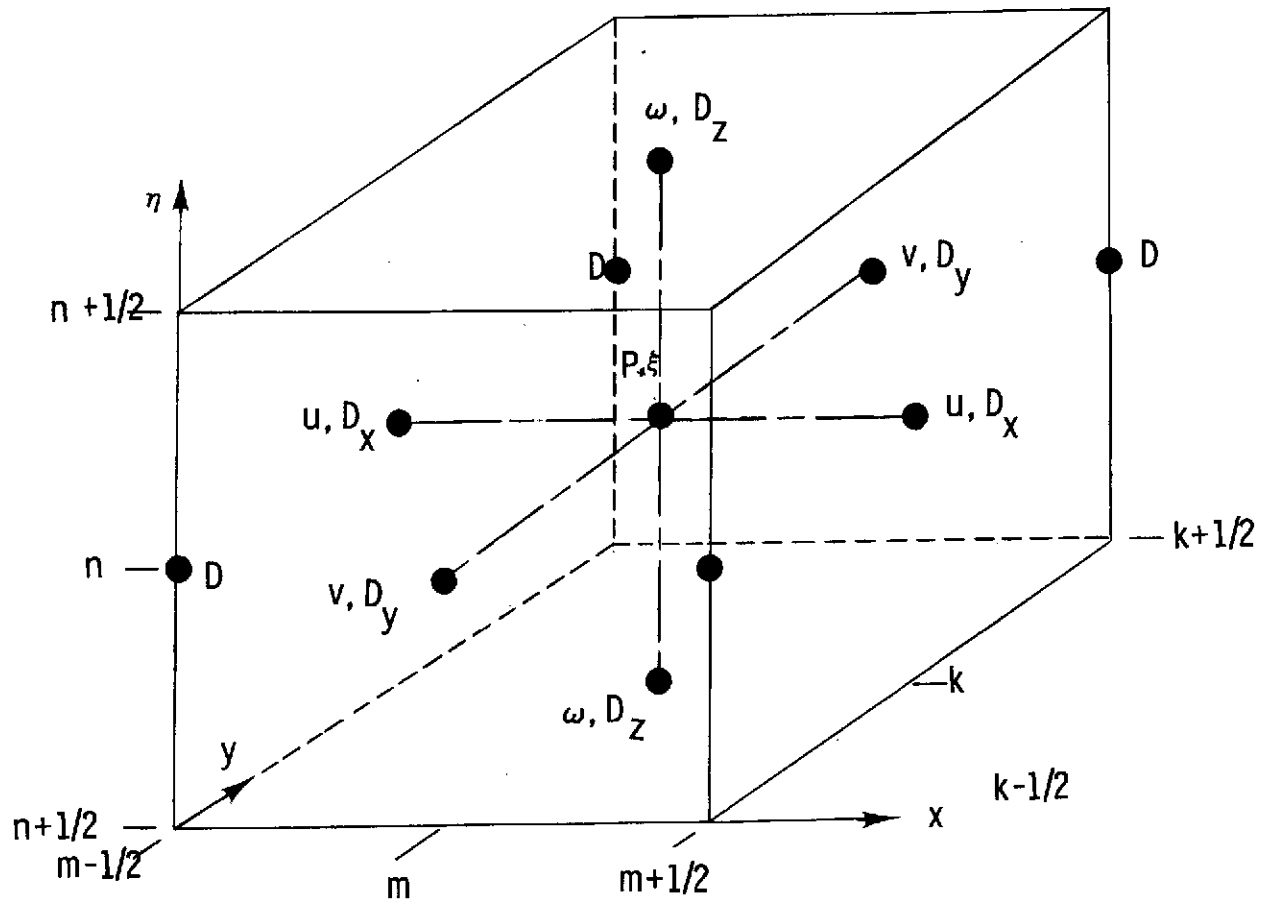


Figure 1. - Coordinate system orientation.



D - Estuary mean sea level depth

ξ - Tidal height

u, v, ω - Velocities in the x, y, and η directions respectively

P - Mass density

D_x, D_y, D_z - Dispersion coefficients for the x, y, and η directions respectively

Figure 2. - Space staggered grid system for 3-D mass transport finite difference approximation.

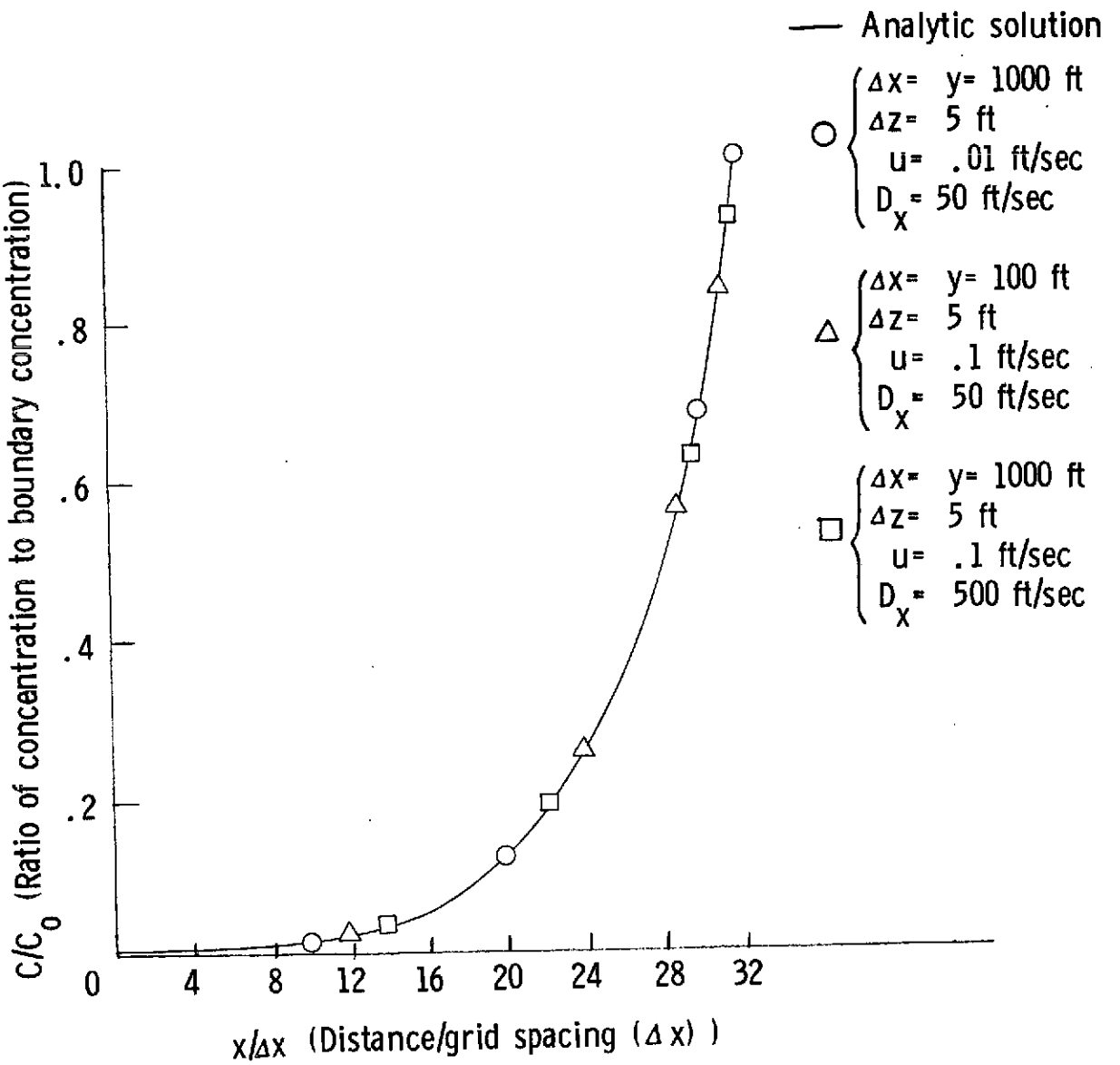


Figure 3. - Comparison of numerical steady-state with analytical solution for 1-D constant velocity and dispersion. Uniform channel flow