

## Digital Simulation of Estuarine Water Quality

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*Abstract.* Partial differential equations describing the unsteady, one-dimensional mixing process in an idealized homogeneous, linearly expanding estuary are presented and solved numerically, using an implicit finite-difference scheme. These solutions portray the change in concentration of conservative substances with time and distance as a result of tidal fluctuations and variable inflow. Although the model presented is highly simplified in terms of estuarine geometry, experiments with varying boundary conditions can provide insight into the adequacy of the more commonly used quasi-steady-state models.

### INTRODUCTION

Impurities introduced into estuarine water are mixed and gradually diluted by fresh water inflow, tidal action, and diffusion. Control or management of estuarine water quality requires a mathematical model that can quantitatively predict the effects of changes in location, amounts, and timing of waste discharges. The structure of the model will depend largely on the nature of the problem. If transients are of no importance, then stationary solutions with boundary conditions described by periodic functions are adequate. On the other hand, an unsteady model appears desirable if one considers the following examples as management possibilities confronting a control agency concerned with estuarine water quality:

1. The operation of a waste treatment plant may be cycled such that its discharges will coincide with the variations in tidal currents that result in the most efficient transport of wastes out to the sea.
2. A water intake may be operated to withdraw water of the highest quality possible during the cyclical water quality fluctuations imposed by the tides.
3. The short-run operation of a water-related facility may be modified when an intense, short-

duration storm strikes the area and causes rapid deterioration of water quality.

The purpose of this paper is to present a mathematical model that simulates the non-steady hydrodynamic behavior of an estuary and to incorporate this into a model that predicts the dispersion of a conservative impurity in estuarine waters. It was anticipated that numerical experiments carried out on such a model could provide insight into the adequacy of the more commonly used quasi-steady models.

### THE HYDRODYNAMIC MODEL

The motion of tidal waters is caused not only by gravity and tidal action, but also by density currents and wind shear. A realization of the complex nature of the driving forces leads to the conclusion that it is desirable to make some compromise between the completely rigorous mathematical formulation and the practical necessity of building a workable model. The simplifying assumptions introduced must be consistent with prototype conditions for a valid model.

The proposed model is typical of several estuaries located on the eastern seaboard of the United States, and its practical application in each of these cases is not diminished by the

general, rather than specific, approach taken herein. The following assumptions apply to the flow equations that were used:

1. The channel has a rectangular cross section, linearly diverging sides for which the rate of divergence is sufficiently small to approximate unidirectional flow at any cross section, and constant bed slope, sufficiently small that the sine of the angle of slope may be taken to be equal to the tangent and the cosine to be equal to unity.
2. The flow velocity is uniform over any cross section.
3. The fluid is of homogeneous density throughout.
4. The energy losses resulting from boundary drag and turbulence can be accounted for by a resistance factor that is determined from the slope of the energy gradient; the resistance factor for uniform, steady flow may be applied

to nonuniform, unsteady flow of the same depth and average velocity.

5. The flow is subcritical at all times.

The model estuary adopted for this analysis is displayed in Figure 1; the following notation will be utilized:

1.  $x$ , the longitudinal coordinate system whose origin is taken at the upstream boundary;
2.  $h$ , the water depth, a function of  $x$  and time only;
3.  $u$ , the velocity of flow, a function of  $x$  and time only;
4.  $L_0$ , the length of the estuary;
5.  $B_0$ , the width of the channel at the upstream boundary;
6.  $b$ , the expansion rate of the channel sides;
7.  $B$ , the channel width, related to  $x$  by the following expression:

$$B = B_0 + bx$$

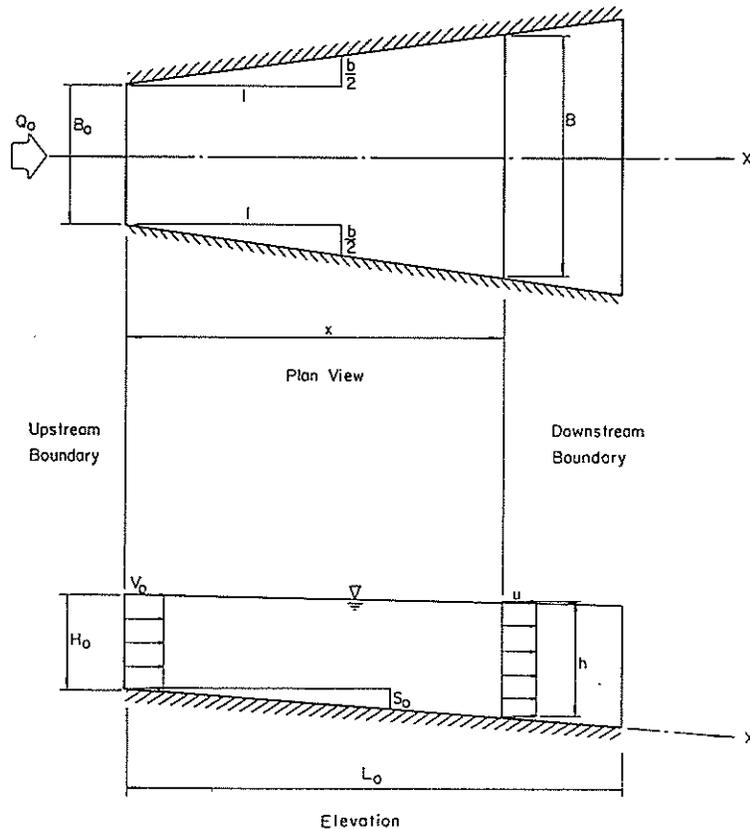


Fig. 1. Idealized estuary.

8.  $S_0$ , the bed slope;
9.  $Q_0$ , the mean river discharge into the estuary;
10.  $H_0$ , the normal water depth at the upstream boundary at discharge  $Q_0$ .
11.  $V_0$ , the normal velocity at the upstream boundary at discharge  $Q_0$ .

#### THE EQUATIONS OF FLOW

By writing the equations of flow in non-dimensional form, it is possible to apply a given solution to many flow conditions by selecting convenient reference quantities and defining the dimensionless variables by the following ratios:

$$x_* = x/L_0 \quad h_* = h/H_0 \quad u_* = u/V_0$$

$$t_* = tV_0/L_0 \quad B_* = B/B_0 = 1 + bx/B_0$$

where the subscript 0 designates a reference quantity, and  $t$  represents the independent variable time.

Substituting the above dimensionless quantities into the continuity and momentum equation for unsteady free-surface flow in an expanding section, we obtain the following dimensionless expressions:

The dimensionless equation of continuity

$$u_* \frac{\partial h_*}{\partial x_*} + h_* \frac{\partial u_*}{\partial x_*} + \frac{L_0 u_* h_* b}{B_0 B_*} + \frac{\partial h_*}{\partial t_*} = 0 \quad (1)$$

and the momentum equation

$$u_* \frac{\partial u_*}{\partial x_*} + \frac{\partial u_*}{\partial t_*} + \frac{1}{F_0^2} \frac{\partial h_*}{\partial x_*} = \frac{S_0 L_0}{H_0 F_0^2} \left( 1 - \frac{u_* |u_*|}{h_*} \right) \quad (2)$$

where  $F_0$  is a dimensionless Froude number defined by the relation

$$F_0 = V_0 / \sqrt{gH_0}$$

#### SOLUTION OF THE EQUATIONS OF FLOW

The simultaneous solution of the equations of continuity and motion consists of finding the set of functions of  $x_*$  and  $t_*$  which, when substituted in the equations in place of the unknowns  $u_*$  and  $h_*$ , will satisfy them identically. Since the equations are highly nonlinear, the solution can best be obtained numerically.

The equations are typical of initial value problems as discussed by Richtmyer [1957].

The properties of these problems are such that, given the state of the physical system at some initial time  $t_0$ , the solution for  $t$  greater than  $t_0$  is uniquely determined by the above equations and the specified boundary conditions.

#### Finite Difference Forms of the Equations of Flow

The solution technique chosen consists of replacing the partial differential equations and the associated initial and boundary conditions with an equivalent discrete approximation. Thus, the continuous derivatives are replaced by finite difference approximations, and the desired functions are evaluated only at discrete points in the solution domain.

The solution domain is shown in Figure 2 with the finite difference net superimposed; its relationship to the physical situation is indicated. The implicit difference scheme used herein is centered about an imaginary grid point at  $t = i + 1/2$ . The difference scheme used and the algorithm used for solution of the resulting simultaneous equations are essentially the same as those used by Liggett and Woolhiser [1967].

*Initial conditions.* The initial values of  $u$  and  $h$  are difficult to obtain, because of the dynamic condition that exists in an estuary. Therefore, arbitrary initial conditions are selected to conform with the anticipated flow patterns. As the solution progresses through time, the influence of the initial conditions diminishes, and the solution is completely determined by the boundary conditions. When this state is reached, the dynamic flow patterns are properly described, and all succeeding calculations may be performed by redefining the initial conditions to be those final values resulting from the preliminary solution.

*Upstream boundary.* The boundary conditions imposed on the solution of a differential equation describing a physical system vary with the nature of the problem. The two conditions imposed at the upstream boundary are:

1. The height of the water surface is specified as a function of time, the data being available from records of river stages.

2. A condition of antisymmetry is assumed to exist for the variable  $h$ . This has been called a transmission boundary condition by Shamir and Harleman [1967] and guarantees a continuation

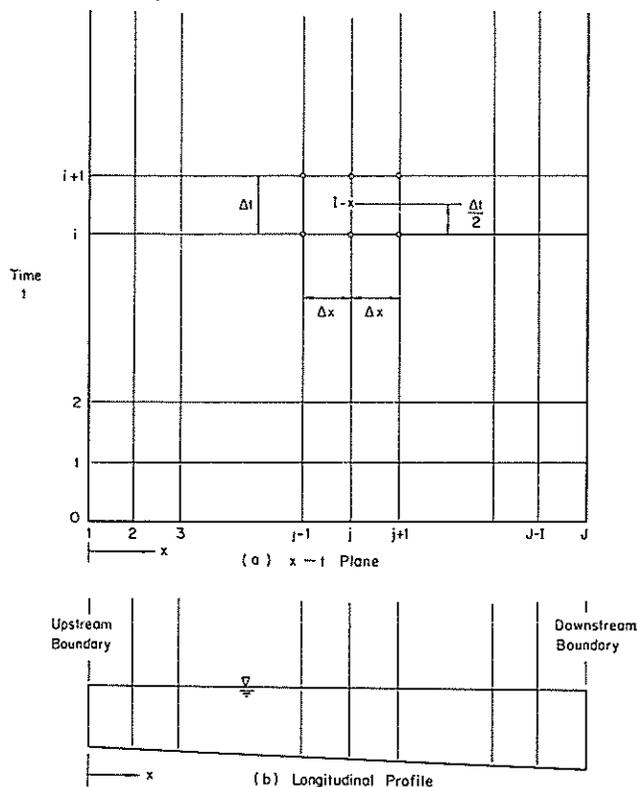


Fig. 2. Solution domain.

of the slope of the water surface through the boundary.

*Downstream boundary.* Tidal fluctuations are imposed on the model at the downstream boundary. The tides were characterized by the single component

$$h = H_D + A_1 \cos(a_1 t + \alpha_1) \quad (3)$$

where  $H_D$  is the height of mean sea level above the channel bed, and the tidal parameters are  $A_1$ , the amplitude or semirange of the simulated tide;

$a_1$ , the speed, which defines the period as  $360^\circ/a_1$ ;

$\alpha_1$ , the initial phase.

The parameters listed are readily available for many coastal locations. The following are prescribed at the downstream boundary:

- (1) The tidal height  $h$ , as given by equation 3.
- (2) A condition of antisymmetry is assumed to exist for  $h$ .

#### ACCURACY AND STABILITY

If  $u(x, t)$  is the exact solution of the initial value problem, and  $u_j^i$  is the solution of the finite difference equations, the error of the approximation is

$$|u_j^i - u(j \Delta x, i \Delta t)|$$

It is desirable to know the behavior of the above error term, as the number of calculation cycles becomes very large, and there is the possibility of unlimited errors due to truncation roundoff or other causes.

For properly formulated explicit schemes, the following Courant condition is imposed on the relative step sizes to prevent these errors from becoming so amplified over  $n$  cycles that the solution is meaningless:

$$\Delta x / \Delta t \geq |u| + C$$

where  $C$  is the wave celerity for the given channel depth.

A linear stability analysis of the implicit scheme used in the study indicated uncondi-

tional stability. However, we observed instabilities in the solutions in some cases. These instabilities were eliminated by reducing the step length. This finding agrees with the work of *Meijer et al.* [1965], who used an implicit scheme for solving a simplified form of the same equations.

An implicit scheme was adopted for this study because of its theoretically stable nature and because several explicit schemes had been unreliable for the overland flow problem [*Liggett and Woolhiser, 1967*]. Since this work was completed, the group at Delft, who have had a great deal of experience with estuary and river problems, have used explicit methods very successfully. They have shown that the apparent unreliability of some of the conditionally stable explicit methods was caused by the manner in which the friction term was handled in discrete form [*Vreugdenhil, 1966*]. Consequently, the use of explicit schemes for this problem should

not be dismissed, as they have many advantages where the channel geometry is complex.

VERIFICATION OF THE SOLUTION

*Liggett* [1961] presented a method for computing open-channel profiles for steady, non-uniform flows. Figure 3 presents a test case solution resulting from the proposed hydrodynamic model operated under steady-state boundary conditions as compared with the solution obtained by *Liggett*. From this comparison we concluded that the hydrodynamic model and the finite-difference algorithm were acceptable.

THE DISPERSION MODEL

Mass transport in tidal waters involves three basic mechanisms:

1. Advection, the time-smoothed mass average flow resulting from the bulk fluid velocity;

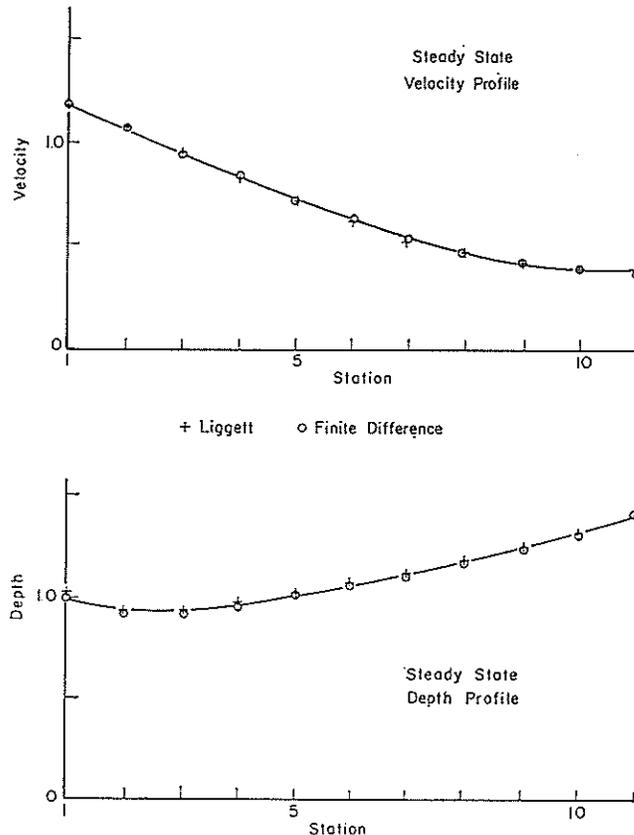


Fig. 3. Verification of the hydrodynamic model.

2. Turbulent diffusion, the fluctuating mass flow resulting from the local fluid velocity;

3. Molecular diffusion, the random migration of individual molecules resulting from their kinetic energy.

The model presented herein is based on those mixing processes characteristic of an unstratified type-D estuary, as outlined by Pritchard [1955]. The simplifying assumptions involved are:

1. The mechanism of turbulent diffusion is analogous to that of molecular diffusion and obeys Fick's Law;

2. Molecular diffusion is negligible when compared with turbulent diffusion and advection;

3. Advective and diffusive transport occur only in the longitudinal direction.

4. The concentration of contaminant is uniform in the vertical and lateral directions at any cross section.

The parameters of the conservation equation are those presented previously, with the following additions:

1.  $c$  is the concentration of contaminant, a function of  $x$  and time only;

2.  $\partial c/\partial x$  is the longitudinal concentration gradient;

3.  $C_0$  is the mean concentration value at that station along the channel where concentration is a maximum.

4.  $E$  is the longitudinal coefficient of turbulent diffusivity and is assumed to be a function of  $x$  only.

The conservation equation is constructed from a materials balance on the element under consideration. The equation states that the net rate of mass flux into and out of the element, plus that produced at the sources during a small interval of time  $dt$  must equal the time rate of change of mass within the element.

*Mass balance equation in nondimensional form.* The nondimensional form of the conservation equation is obtained by utilizing the dimensionless variables defined previously and introducing the following ratios:

$$c_* = c/C_0 \quad E_* = E/(L_0 V_0)$$

The mass balance equation in its final form

becomes

$$\begin{aligned} E_* h_* \frac{\partial^2 c_*}{\partial x_*^2} + \left( -u_* h_* + h_* \frac{\partial E_*}{\partial x_*} \right. \\ \left. + E_* \frac{\partial h_*}{\partial x_*} + E_* \frac{L_0 b h_*}{B_0 B_*} \right) \frac{\partial c_*}{\partial x_*} \\ + \left( -u_* \frac{\partial h_*}{\partial x_*} - h_* \frac{\partial u_*}{\partial x_*} \right. \\ \left. - u_* h_* \frac{L_0 b}{B_0 B_*} - \frac{\partial h_*}{\partial t_*} \right) c_* = h_* \frac{\partial c_*}{\partial t_*} \quad (4) \end{aligned}$$

The method of solution of the mass balance equation, a typical initial value problem, very nearly parallels that outlined for the flow equations. The grid system employed is identical with that used previously. The values of  $u_*$  and  $h_*$  are now known and are used to evaluate the coefficients of the conservation equation.

An implicit difference scheme, centered at  $t = i + 1/2$ , was employed to write the mass balance equation in finite difference form. A preliminary solution was performed utilizing arbitrary initial conditions and allowing the transient response to die away. The resulting unsteady concentration profile served as the initial condition for all succeeding computations.

The basic simulation model developed was used to investigate the following cases:

1. The salinity profiles resulting from the intrusion of sea water;

2. The dispersion pattern resulting from a continuous waste discharge;

3. The dispersion pattern resulting from a slug waste discharge.

#### SEA WATER INTRUSION MODEL

*Upstream boundary:* The condition states that the concentration of salt at the upstream boundary must equal zero; this is consistent with the fresh water inflows at the head of the estuary.

*Downstream boundary:* The downstream boundary was constructed at a fictitious point 0, a distance  $D$  beyond the mouth of the estuary. The concentration of salt at point 0 is equal to that of sea water  $C_0$ . If the concentration of salt at the mouth were specified as that of sea water, it would imply that the fresh water inflows to the estuary do not exert a dilution effect at the mouth. The imaginary boundary

used herein allows for possible concentration fluctuations at the entrance while assuring a constant concentration farther out to sea.

THE CONTINUOUS WASTE DISCHARGE MODEL

*Upstream boundary.* An antisymmetry condition was specified at the upstream boundary, justified by assuming that the variable concentration at the boundary would remain small, and hence that the curvature of the concentration profile would be negligible.

*Downstream boundary.* The downstream boundary was constructed at a fictitious point 0, as discussed previously. The reasoning for constructing such a boundary in this case is similar; waste concentrations do not approach an infinite dilution at the entrance to the estuary, but rather at some distance farther out to sea. Thus,

the concentration at point 0, a distance  $D$  from the mouth, is zero for all time.

*Internal boundary.* If discharge is continuous, an internal boundary condition is necessary. This boundary is permanently located at the station nearest the outfall and consists of the concentration of contaminant at the outfall station. This concentration is computed from an inventory equation covering the entire estuary.

SLUG WASTE DISCHARGE

*Upstream boundary.* The upstream boundary was identical with that specified for the continuous discharge model.

*Downstream boundary.* The downstream boundary also was identical with that prescribed for the continuous discharge model.

*Internal boundary.* An internal boundary is

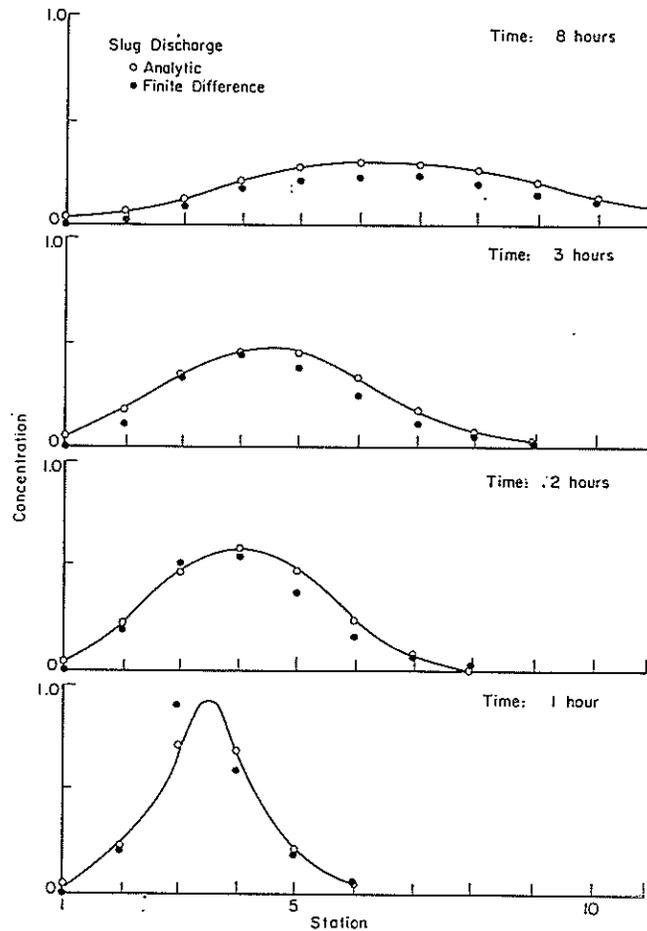


Fig. 4. Verification of the dispersion model.

necessary to trace the motion of a slug of contaminant in the estuary. This boundary is located at the modal value of concentration of contaminant and is initially at the station nearest the outfall. However, it is translated through the estuary by the unsteady tidal currents. The value of concentration to be specified is then determined by the inventory procedure mentioned previously.

ACCURACY AND STABILITY

The dispersion model did not exhibit instabilities for the mesh sizes used; these mesh sizes, however, were governed by the step size imposed on the hydrodynamic model.

*Verification of the Solution:* A closed analytic solution [Kent, 1960] exists for the one-dimensional mass balance equation if the following simplifications apply:

1. Steady, uniform flow with velocity  $\bar{u}$ ;
2. A slug of conservative contaminant is instantaneously discharged at one point in the channel;
3. Diffusion and advection are the only forms of mass transport. The form of the solution is

$$c(x, t) = \frac{A}{t^{1/2}} \exp\left(\frac{-(x - \bar{u}t)^2}{4Et}\right)$$

where

$$A = \frac{1}{2(\pi E)^{1/2}} \int_{-\infty}^{\infty} c \, dx$$

Figure 4 compares the analytic solution with the values resulting from model simulation of the same problem. The agreement was satisfactory over the range of  $x$  and  $t$  studied.

RESULTS

*General.* The model was programmed in the Fortran 63 language, and the computations were performed on a Control Data 1604 Computer. The hydrodynamic model and the three dispersion models were written as separate sub-routines; therefore, one may assemble the desired components to suit the particular problem under investigation.

Approximately one minute of computer time is necessary to simulate 24 hours of data for a single water quality parameter. The results, presented in graphical form, can be readily examined for long-term and short-term trends in water quality.

APPLICATION I: A HYPOTHETICAL ESTUARY

The capabilities of the unsteady model are demonstrated by simulating water quality in a

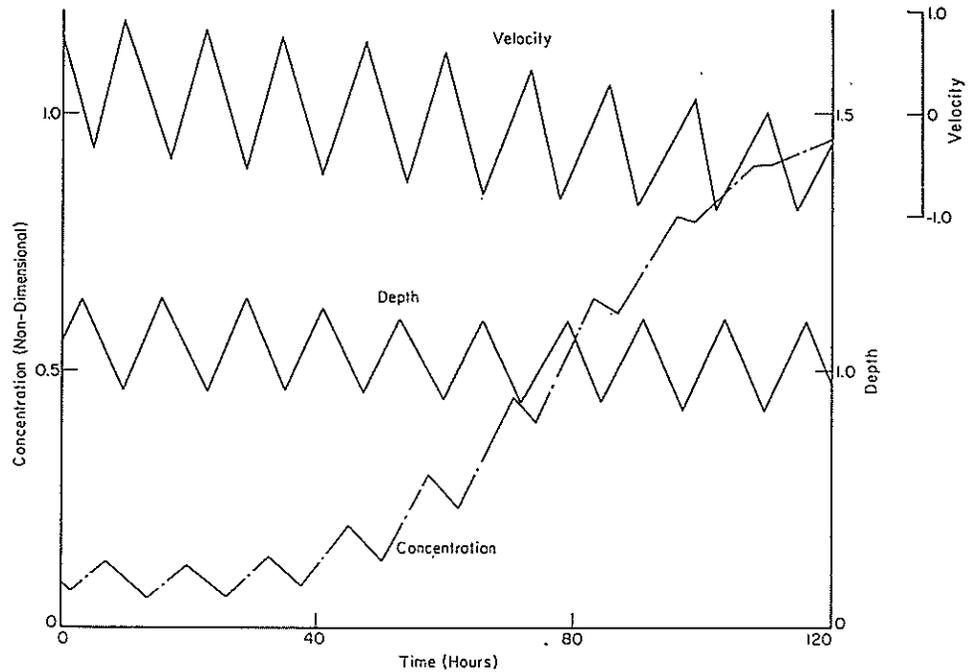


Fig. 5. Salt intrusion, low flow conditions, profile at Station 7.

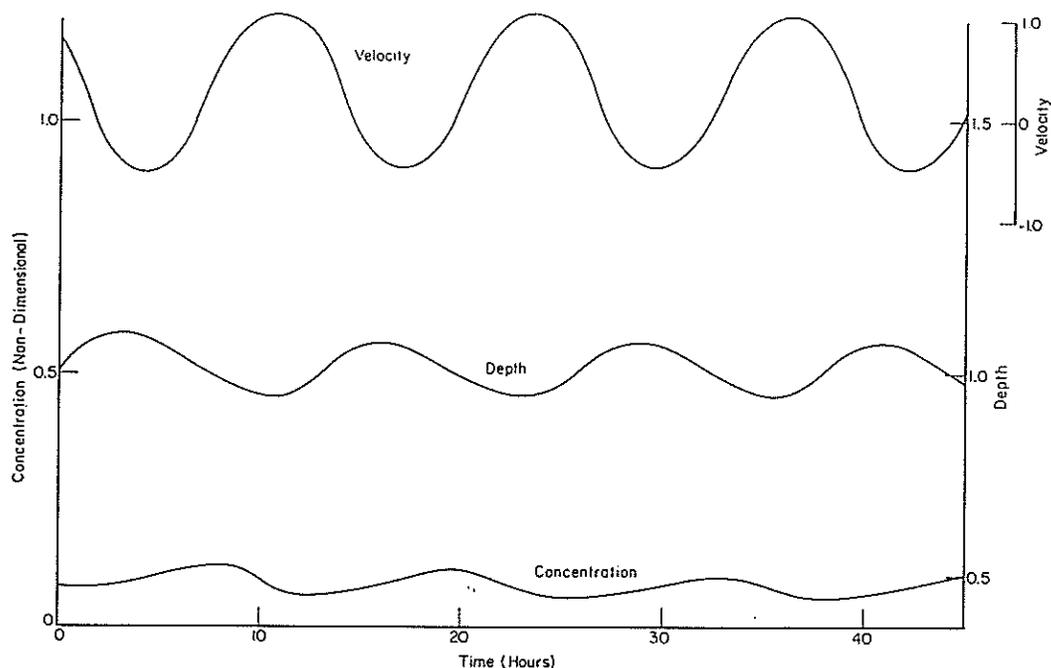


Fig. 6. Continuous discharge mean flow conditions, profile at Station 4.

hypothetical estuary whose parameters are given as

$$\begin{array}{ll}
 L_0 = 158,400 \text{ ft} & H_0 = 20.0 \text{ ft} \\
 B_0 = 2,000 \text{ ft} & H_D = 20.0 \text{ ft} \\
 b = 0.018 & A_1 = 2.0 \text{ ft} \\
 S_0 = 0.00002 & a_1 = 28.91^\circ/\text{hr} \\
 Q_0 = 80000 \text{ cfs} & \alpha_1 = 0 \\
 V_0 = 2.0 \text{ fps} & E = 24-48 \text{ sq mi/day} \\
 C_0 = 1.0 \text{ ppm} &
 \end{array}$$

The mesh size chosen was:  $\Delta x = 0.1$   $\Delta t = .0091$ . The ratio  $\Delta x/\Delta t$  did not produce signs of instability.

The results presented are:

1. Salt intrusion under low flow conditions. Figure 5 shows the time variation of salt concentration at station 7 as the fresh water inflow is gradually diminished to one-half the mean flow value. Only the peaks and valleys of concentration depth and velocity are plotted in Figure 5. Actually, there were about 15 points between each of those on the figure.

2. Continuous waste discharge. Figure 6 shows the time variation of concentration at the outfall for mean flow conditions.

3. Slug waste discharge. Figure 7 shows the

time variation of concentration at the outfall for mean flow conditions.

#### APPLICATION 2: THE DELAWARE ESTUARY

The assumptions on which this model is based were found to approximate roughly prototype conditions in the Delaware Estuary. One method of evaluating the practical performance of the model is to compare recorded observations with model predictions.

The values of parameters used to describe the Delaware Estuary from Trenton, New Jersey to Reedy Island, Delaware, are

$$\begin{array}{ll}
 L_0 = 450,000 \text{ ft} & H_0 = 18.0 \text{ ft} \\
 B_0 = 600 \text{ ft} & H_D = 18.0 \text{ ft} \\
 b = 0.019 & A_1 = 2.5 \text{ ft} \\
 S_0 = 0.00001 & a_1 = 28.91^\circ/\text{hr} \\
 Q_0 = 16,000 \text{ cfs} & \alpha_1 = 0 \\
 V_0 = 1.48 \text{ fps} & E = 5-15 \text{ sq mi/day}
 \end{array}$$

This attempt did not succeed, however, because of serious problems with the hydrodynamic model. Figure 8 shows that the steady-state discharge profile clearly violates continuity, in that upstream inflow is 51,854 cfs and the downstream discharge is 59,637 cfs.

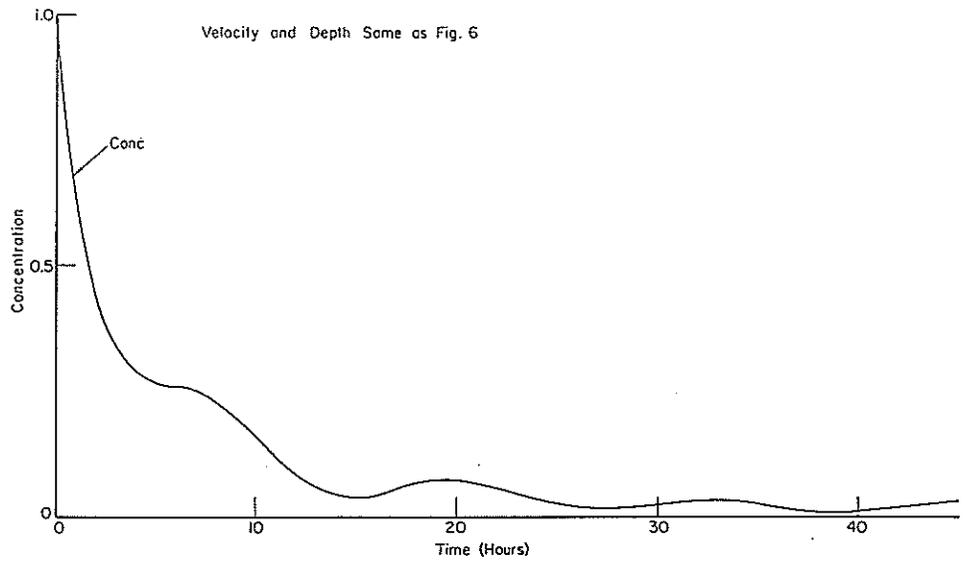


Fig. 7. Slug discharge, mean flow conditions, profile at Station 3.

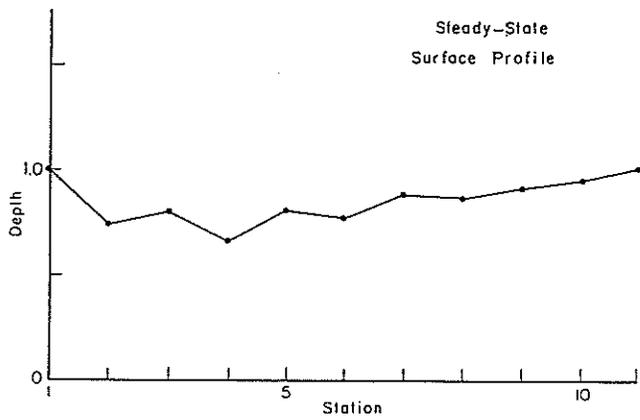
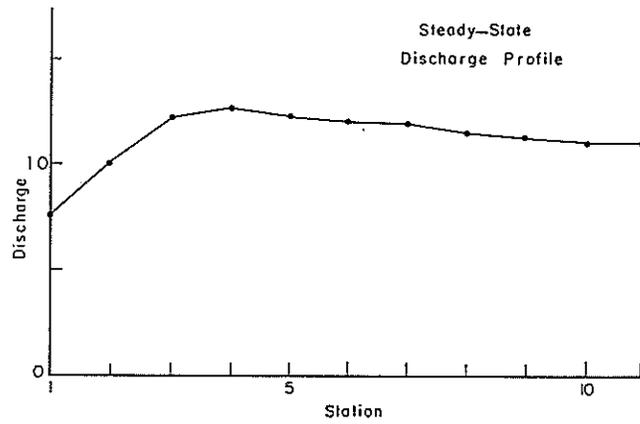


Fig. 8. Delaware estuary profiles.

The boundaries came under suspicion and were investigated more thoroughly. In particular, the antisymmetry condition was questioned. For this purpose the Method of Characteristics must be introduced. *Stoker* [1963] discussed the theory involved, and *Veal* [1966] presented an application closely related to the model study in this thesis.

The characteristic solution requires that only a single parameter be specified at the boundary, either  $h$  or  $u$ , or a unique relationship between them. Assuming that the depth is specified at both boundaries, the antisymmetry condition becomes mathematically redundant and may introduce errors when curvature is present.

To verify whether or not this was the source of the error, a steady-state model solution was obtained by imposing the correct steady-state profile as initial conditions. The results are shown in Figure 9 and confirm the above hypothesis. The solution within zone A, influenced solely by the initial conditions, remains unchanged from the correct values, indicating stability in the finite difference scheme. The remainder of the solution, affected by the steady boundary conditions, shows the fluctuations propagated in from the boundaries.

CONCLUSIONS AND RECOMMENDATIONS

The differential equations incorporated in the estuary model proposed in this paper are based on sound physical principles. The difficulties that appeared in simulating the Delaware Estuary apparently stemmed from the assumed condition of antisymmetry at the boundary. This approximation was poor for the Delaware Estuary because of the significant amount of curvature in the depth profile at the upstream boundary.

Future work should concentrate on validating the model—as an example, the verification attempted herein using the Delaware Estuary. The difficulties associated with the antisymmetry boundary condition may be eliminated by using a characteristic solution at the boundaries. In joining the irregular characteristic net with the rectangular implicit net used for the interior points, certain interpolation errors will result, especially where curvature is significant. However, it is felt that the characteristic solution is preferable to assuming antisymmetry at the boundaries.

Extension of the model to simulate estuaries with tributary inflows, nonlinear variations in channel widths and slopes, and multiple outfalls

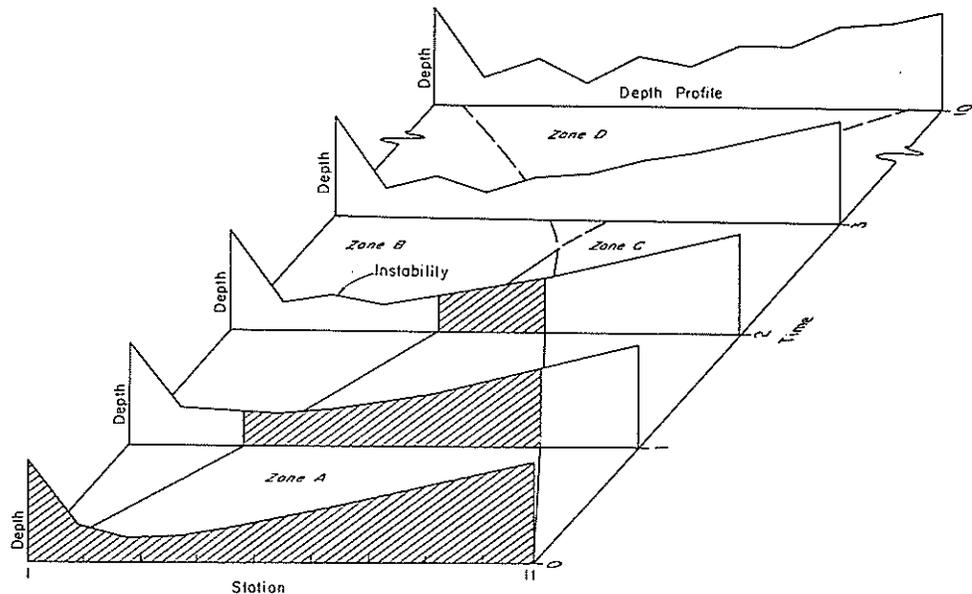


Fig. 9. Zone A solution.

is readily possible by virtue of the finite difference solution used to solve the differential equations.

The nondimensional parameters of the solution  $F_0^2$ ,  $(S_0 L_0)/(H_0 F_0^2)$  and  $(L_0 b)/B_0$  permit an investigation of the effect of parameter variation on water quality that requires only a fraction of the number of trials necessary when dimensional equations are employed.

A natural extension of this problem would be a model for predicting concentration profiles for nonconservative substances. It is recognized, however, that there is very little information available on the nature of decay processes in unsteady tidal streams, and that research in this area is essential if mathematical models are to be relevant to real problems.

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