

CHAPTER 129

A NUMERICAL MODEL OF ESTUARINE POLLUTANT TRANSPORT

by

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I. INTRODUCTION

Pollutant transport studies in estuaries may be divided into two general types: firstly, those where a new pollutant will be discharged into an existing estuary; and secondly, those where the estuarine geometry will be changed permanently. The first type of problem is analyzed more easily because distributions of existing natural or artificial tracers can be used to determine rates of transport and diffusion. For this type of problem one-dimensional or time-averaged two-dimensional models, employing apparent diffusivities evaluated from existing tracers, are often satisfactory. When permanent changes in the system are envisaged, however, it is likely that the bulk or apparent diffusivities of space and time-averaged models will be changed in unpredictable ways. Hence to determine what will be the effect of dredging a new channel in an estuary, or permanently changing the distribution of fresh water inflow, more sophisticated models must include the underlying mechanisms of pollutant transport and diffusion. The purpose of this paper is to present a two-dimensional, non-time averaged model which is computationally fast, seems to be reasonably accurate, and can be used to predict the effect of permanent changes wherever a two-dimensional representation is satisfactory.

II. THE CONCEPT OF TWO-DIMENSIONAL MODELING

A computer program to solve the equations of motion and diffusion in three space dimensions and time for a real estuary is beyond the capacity of present day computers. Hence all computer models of estuaries are based on averaging, either over one or two space dimensions, or time, or both. The two-dimensional models discussed herein average only over the vertical dimension, so that the velocity and concentration are considered to be functions of the two horizontal dimensions x and y and time t , but not of the vertical dimension z . The equations to be solved are the vertically-integrated equation of motion,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - fv + g \frac{\partial h}{\partial x} + g \frac{u \sqrt{u^2 + v^2}}{C^2 h} = \frac{\tau_x}{\rho h} \quad (1)$$

in the x direction, and a similar equation in the y direction, and the advective diffusion equation for a dissolved constituent,

$$\frac{\partial(ch)}{\partial t} + \frac{\partial}{\partial x}(uch) + \frac{\partial}{\partial y}(vch) = \frac{\partial}{\partial x} \left(D_x h \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_y h \frac{\partial c}{\partial y} \right) \quad (2)$$

In these equations u and v are velocities and D_x and D_y are diffusivities in the x and y directions, respectively, C is the Chezy coefficient, f is the Coriolis parameter, h is depth, τ_x is the x-component of the wind stress, and c is the concentration of a dissolved substance.

The restrictions on this concept are apparent. u and v are depth averaged velocities, so the velocity profile both in magnitude and direction is resolved into a single, depth averaged vector. The wind stress, which in the prototype exerts a stress on the water surface and produces a vertical, spiraling velocity profile, is resolved into an apparent body force inversely proportional to depth. The dispersive effect of the vertical velocity profile has to be expressed by the diffusivities D_x and D_y , which are therefore not turbulent diffusion coefficients at all, but rather dispersion coefficients depending on the direction, magnitude, and distribution of the velocity vector.

III. DESCRIPTION OF THE MODEL

The model to be described in this report is a two-dimensional model for use in large bays and estuaries with substantial open areas, where stratification is not important. The model is in two parts: first, a solution of the equations of motion, using the finite difference method given by Leendertse (1967); and second, a model for constituent transport developed by the writer and described in detail with a complete listing of the numerical program by Fischer (1970).

The hydrodynamic program is run first, and is operated until steady state is obtained (usually in the second tidal cycle). The x and y components of velocity at each grid point are stored on magnetic tape at hourly or half-hourly increments. This part of the procedure is similar to that used by Leendertse and Gritton (1971, a,b) in a modeling study of Jamaica Bay. Leendertse and Gritton have also developed and used a finite difference solution of the advective diffusion equation, using the same time step as for the hydrodynamic solution. In the present model, however, an alternate method is used, based on the method of superposition, which allows a substantially longer time step. The method of superposition, also called the convolution integral, states that in steady uniform flow the solution to Equation 2, given a known concentration distribution at $t = 0$, is

$$c(x,y,t) = \iint_A \frac{c(\xi,\eta,0)}{4\pi t \sqrt{D_x D_y}} e^{-\frac{1}{4t} \left\{ \frac{(x-ut-\xi)^2}{D_x} + \frac{(y-vt-\eta)^2}{D_y} \right\}} d\xi d\eta \quad (3)$$

This equation gives the concentration distribution resulting from any initial distribution after an arbitrarily long time, in the absence of boundaries. So long as the velocities remain constant there is no limit on the length of time step, and the accuracy of the solution depends only on the accuracy of the numerical integration.

In practice, of course, velocities in estuaries are neither steady nor uniform, and irregular boundary conditions must be satisfied. Furthermore, evaluation of the integral in Equation 3 is time consuming, even on modern numerical equipment, when many grid points are involved. The numerical scheme developed to satisfy these considerations, while still preserving the spirit of the method of superposition and taking advantage of its long time step, is illustrated in Figure 1. In place of the terms $u t$ and $v t$, we use the approximations $\int_0^t u \, dt$ and $\int_0^t v \, dt$, where the time interval may be anything up to the time required for one tidal inflow or outflow. The integration is done in half-hourly steps, using the velocity field generated by the hydrodynamic program. The spatial integration in Equation 3 is replaced by a summation over a limited area, to increase computational speed. The scheme illustrated by Figure 1 uses a 5 point top hat distribution; to compute the concentration at the grid point I,J shown at the end of the path of arrows in Figure 1, we integrate the velocity field backwards in time to locate the closest grid point of origin, M,N, shown as the origin of the path or arrows. $c(I,J)$ is computed by the relationship

$$c(I,J) = 1/5 \{ c(M,N) + c(M+1,N) + c(M-1,N) + c(M,N+1) + c(M,N-1) \} \quad (4)$$

The boundary conditions of inflow from a river, or from the ocean, and the condition at the land boundary, are satisfied as follows. If the back calculation of the velocity field carries an indicator particle into the ocean, it is assigned the ocean concentration. Similarly, if a particle is carried into the river, it is assigned the river concentration, which may be a function of time given by another program. Obviously, no concentrations will be computed for points which are in fact on land; if, by chance, back integration of the velocity field carries the indicator particle out of the water field, its motion is stopped for the remainder of that time step, and it is assigned the nearest water concentration. Hence, all concentrations in the water field are computed by averaging concentrations around the grid point where the particle begins its motion. Diffusion, which is accomplished by the spatial integration of Equation 3, is carried out by the averaging procedure given in Equation 4. The magnitude of the apparent diffusivities, D_x and D_y , can be varied by varying the details of the averaging process, the time step, and the grid spacing. The 5 point averaging scheme shown in Equation 4 and Figure 1 is equivalent to selecting equal diffusivities D_x and D_y equal to $0.2 (\Delta x)^2 / \Delta t$, where, Δx is the distance between grid points and Δt is the duration of the advective time interval. The factor 0.2 is established by the probabilities of the diffusive motion, which in each direction during each time interval are 0.2 one step forward, 0.2 one step backward, and 0.6 no net motion. These probabilities could, of course, easily be changed by revising the averaging given in equation 4.

IV. AN EXAMPLE APPLICATION

The model has been applied to Botany Bay, New South Wales, Australia, as part of a major water quality study of the Georges River-Botany Bay system. The Georges River itself was modeled in one-dimensional segments, using the scheme described by Fischer (1972). Botany Bay is the downstream end of the river, and is a roughly circular embayment approximately three miles in diameter. The model was used to study the present geometry, and also a proposed geometry including a breakwater and port development. A one thousand foot grid was used, and an observed tide at the mouth of the bay was simulated. The model computed tidal elevations and velocities and the concentrations of six constituents throughout the bay and river system.

Figure 2 shows a typical example of currents computed in Botany Bay. These currents are used in the water quality model, and Figure 3 shows a typical result for a non-conservative constituent. Three constituent sources were modeled: the ocean, the Georges River, as a time-varying source computed by the river model, and a point source at the Cooks River. At the ocean mouth, a tidal exchange ratio of 75% was assumed. This was distributed over the tidal cycle by assuming that in the first hour of tidal inflow 50% of the inflowing water had just left on the previous tide, in the second hour 25%, and thereafter, zero. Wind stresses from winds coming from several directions were assumed, although in the simple geometry of Botany Bay wind driven circulations did not appear to be of major importance.

The model was first used to model salinity, because verification of a salinity distribution provides a good check on the physical description of the system. The salinity distribution in the Georges River was modeled with reasonable accuracy for a range of river discharges; unfortunately, this did not provide verification of the model in the bay, because the salinity within the bay is nearly constant. After the model was verified for salinity, concentrations were computed for biochemical oxygen demand, dissolved oxygen, coliforms, phosphorous, and nitrogen. To the extent that field data were available, reasonable verifications were obtained for all constituents.

V. DISCUSSION OF RESULTS

The water quality model presented herein represents a departure from the usual finite difference numerical method. The new method is always stable, by virtue of the method of averaging, and will always yield results which at least appear to be reasonable. When a very long time step is used the accuracy does, of course, suffer; in the present study, which used a six to eight hour time step, some of the details of the tidal flow were lost. On the other hand, the longer time step has the major advantage of permitting simulation of longer periods at reasonable cost. This is particularly important for water quality models, because while a hydrodynamic steady state may be achieved within two or three tidal cycles,

a steady state distribution of a constituent often requires as much as 30 to 60 tidal cycles, depending upon the size of the system. Ward and Fischer (1971) found, for example, that in the Delaware estuary a 30 day equilibrium time might be reasonable, and Hyer (1972) found that in some hydraulic model experiments 30 to 60 days were required to reach a salinity equilibrium. Thus, an important requirement for a water quality numerical model is an ability to run for 30 to 60 tidal cycles at reasonable cost.

In the present model, turbulent mixing both in the flow direction and transverse to the flow direction is simulated by mixing over a radius of 1000 feet at the end of every tidal inflow or outflow. This corresponds to assuming values of the turbulent mixing coefficients of approximately $10 \text{ ft}^2/\text{sec}$. in each direction. These coefficients actually represent the effect of velocity shear in all directions, and their magnitudes in real estuaries are not well known. For dispersion in the flow direction, one can obtain the magnitude of the coefficient by using Elder's result $D_x = 6 d u^*$ where d is the depth of flow and u^* is the shear velocity. For Botany Bay, this would yield a value of the order of $10 \text{ ft}^2/\text{sec}$. In the transverse direction, dispersion is probably caused by a rotation of the velocity vector with depth, as discussed by Ward (1972). Little can be said, however, about the magnitude of the transverse coefficient in real estuaries, as it is affected by a number of factors particular to each individual estuary. The assumption used for mixing in the present model, while very approximate, is probably as accurate a representation of what happens in real estuaries as can be devised from present knowledge. More field data on this aspect of dispersion are essential.

In summary, the model presented in this report represents an attempt to simulate the physical processes of transport and dispersion of constituents in estuaries. The time step used is long, permitting simulation of a long period of real time. Accuracy can probably be improved by shortening the time step and increasing the degree to which the details of convective transport are modeled. The model is presently being applied to several real estuaries and it is hoped that further development will provide a useful tool for water quality studies.

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FIGURE CAPTIONS

Figure 1: Schematic drawing of particle motion in the transport model.

Figure 2: A typical computed velocity distribution in Botany Bay.

Figure 3: Predicted NO_2 and NO_3 levels (mg/l as N) in Botany Bay at low tide, July 1969.





