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THREE-DIMENSIONAL FREE-SURFACE SUSPENDED PARTICLES TRANSPORT IN THE SOUTH BISCAYNE BAY, FLORIDA

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SUMMARY

A three-dimensional, time-dependent free surface model has been developed which takes account of topographical and meteorological parameters for application to suspended particles transport. This investigation of suspended particles transport is the most realistic in regard to treating the moving free-surface in computing the hydrodynamic field. A unique mass-conserving numerical model is used for solving the concentration equation by an explicit finite difference scheme. The paper presents a mathematical model which can be applied to surface water dispersion of particulates associated with dredging operations and land-fill. The effects of settling velocity and bottom bed deposition rate are compared and discussed.

KEY WORDS Hydrodynamic Model Suspended Particles Transport Free-surface Model Bottom Bed Deposition Particle Settling Velocity Particulate Dispersion

INTRODUCTION

A three-dimensional, time-dependent free surface hydrodynamic model has been developed which takes account of topographical and meteorological parameters for the application to suspended particles transport. Suspended particles transport has been treated for application to the South Bicayne Bay.[1]

This paper presents a unique mass-conserving explicit finite difference model for solving the concentration equation for suspended particles transport by invoking both second upwind differencing of the horizontal convection terms, and a control volume integral formulation for the free surface and bottom boundaries. The mass transport model can be directly applied to surface water dispersion of particulates associated with dredging operations and land-fill. The paper presents a bottom bed boundary condition which is a function of vertical diffusion, particle settling velocity, bed deposition probability and the local vertical concentration gradient.

The South Biscayne Bay is a tide dominated shallow bay bordering the City of Miami (Figure 1). Local tidal effects have been introduced into the mathematical model by applying an open boundary condition at the ocean–bay interface.[2] Agreement with a long-term temporally averaged tide data base, both at the ocean exchange area and at several shore-line locations, for a velocity calibrated model on the basis of a velocity current data base, is quite good.[3,4] Previous work by

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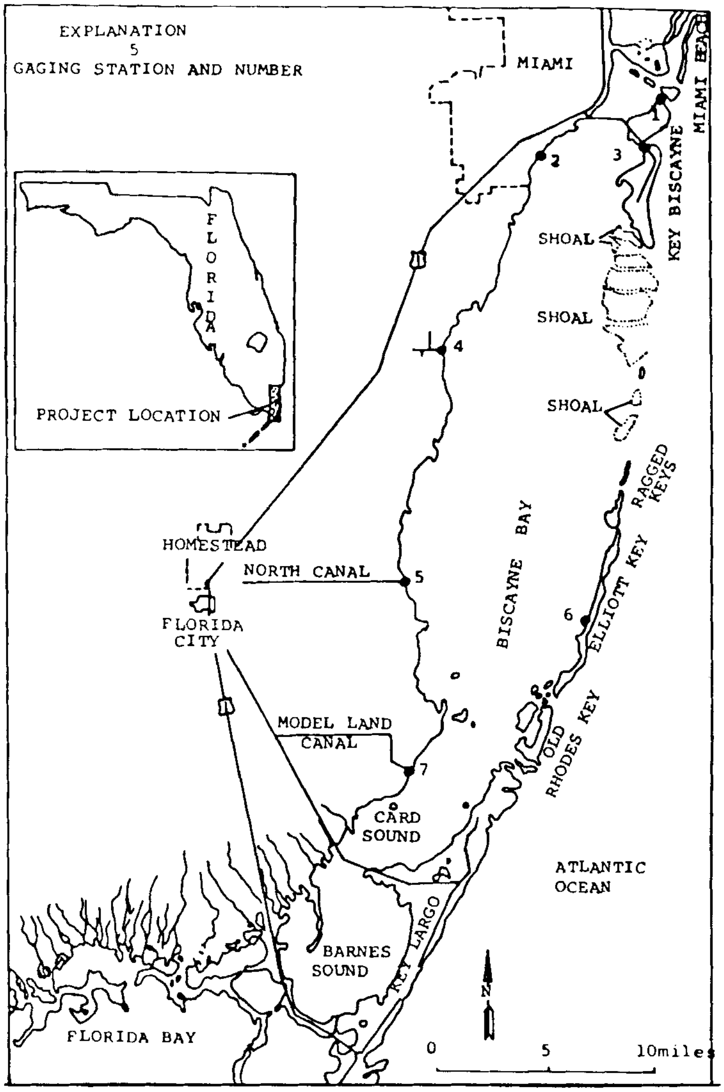

Figure 1. Map of South Biscayne Bay

other researchers[5] has not included the moving free surface, and the exact form of the open boundary condition at the ocean–bay interface has not been used, but has been purely empirical.[6,7] This paper presents an unstaggered grid system for the mathematical model wherein the hydrodynamic equations are directly coupled to the suspended particles transport equation by using a turbulent Schmidt number of unity. This assumption has been justified based upon experimental investigation.[8] The unstaggered grid system has been effectively used in second upwind differencing and in the free surface and bottom boundary equations by defining species concentration cell averages. Hence, for the mass transport, accurate phase speed averaging was achieved.

Miller[9] comments on the tidal phase averaging required in applying the closed form open boundary condition at the bay inlet as used by Sengupta, Lee and Miller[10] in an unstaggered grid.

By using a staggered Richardson lattice, Miller[9] has shown that the exact form of the open boundary condition can be incorporated into the hydrodynamic model, without phase averaging. Also, by ignoring horizontal diffusion terms which are quite small for the South Biscayne Bay, the application of the staggered Richardson lattice reduced computer run time by approximately a factor of 60.[9] However, this faster and more accurate hydrodynamic model was not used in this study, since 90 per cent bottom bed deposition occurred in 2 to 4 hours, and, instead the faster staggered model was used for 30 day dissolved chemical bay flushing numerical studies.[11]

Basic particle transport processes, with associated boundary conditions, have been modelled. General features of the suspended particles transport have been evaluated qualitatively, and the behaviour of the dominant physical mechanisms determined. Further research into other physical processes of suspended particles transport, namely, hindered particle settling, flocculation and bottom bed turbulent entrainment, requires detailed, controlled laboratory experiments and extensive field data collection. Various techniques do exist for measuring sediment concentration both by field instruments and laboratory instruments.[12] Thus, this investigation, like the work of other researchers, limited the physics to ideal gravitational settling, and a bottom boundary condition which neglects turbulent entrainment.[13–16]

THE PHYSICAL MODEL

The various physical processes governing sediment transport in a fluid have been summarized[17,18] as well as the modes of sedimentation deposit on the bed of a water basin. Sheng[5] has investigated contaminant dispersion in the near-shore of large lakes using a three-dimensional, time-dependent numerical model. His approach uses an explicit finite difference method invoking a rigid-lid approximation, whereby free surface variations in space and time are not taken into account. This numerical study extends the work of Sheng by incorporating the free surface variations as well as modelling a more physically appropriate bottom boundary condition.

The effects of ideal particle settling, hindered particle settling, flocculation and bed scour, or viscous turbulent entrainment of sediment particles are discussed in detail by Raudkivi.[18] Empirical relationships have been obtained for hindered particles settling, flocculation and entrainment. However, current research investigations[5,8,13–16] have not accounted for entrainment (or bed scour) in their dispersion models, and have only included particle settling effects in terms of ideal gravitational settling, thus ignoring hindered settling and flocculation. Following Tchen[19] and Lumley[20] the sediment particle is assumed to be so small that its motion relative to the ambient fluid follows Stokes' law of resistance. The eddy diffusion coefficient for the particle is the same as that of the fluid. Sayre[21] concluded that small sediment particles (diameter less than 0·1 mm) with a settling velocity in the Stokes range, very nearly follow the turbulent fluctuations, and consequently, have a diffusion coefficient nearly equal to that of the fluid.

The momentum transfer is related to the particulate mass transfer through the dimensionless turbulent Schmidt number. Jobson's[8] experimental investigation indicated an average turbulent Schmidt number of 1·03. Note that the momentum transport affects the mass transport, but not vice versa, since the effect of suspended particles on the dynamics of the flow can be neglected for sufficiently small Richardson number.[22,23]

THE MATHEMATICAL MODEL

The governing equations for three-dimensional, time-dependent free-surface suspended particles transport have been somewhat simplified by considering hydrostatic behaviour, the Boussinesq approximation, and the description of turbulent transport by constant horizontal eddy coefficients. The vertical eddy transport coefficient was based on a 4/3 power law,[1] such that depth variations were taken into account. Since the South Biscayne Bay is shallow and always well-mixed, hydrodynamically, seasonal variations are of second order importance in terms of particle transport. The turbulent Schmidt number has been set equal to unity.

Lee and Sengupta[24] derived their model equations for the general case of variable density. To map the irregular and time-dependent free surface into a fixed flat surface for easy computation, the vertical co-ordinate was transformed.[25,26]

$$\alpha = x$$
$$\beta = y$$
$$\sigma = \frac{z + \eta(x, y, t)}{H(x, y, t)} \tag{1}$$

Where $H = h + \eta$; σ varies monotonically from zero at the free surface to unity at the bottom boundary. This vertical co-ordinate transformation results in a constant depth geometry with a flat free surface in the new co-ordinate system, such that that triplet (α, β, σ) is mutually orthogonal. The hydrodynamic model equations in (α, β, σ) are summarized by Sengupta, Lee and Miller,[1] where higher order terms in (α, β, σ) have been appropriately neglected, for a shallow bay with an integration time step quite small compared to the tidal cycle.

Suspended particles transport equation

The governing equation for mass transport for a finite settling velocity, W_s, for suspended particles in (α, β, σ) is given as

$$\frac{\partial(HC)}{\partial t} + \frac{\partial(HuC)}{\partial \alpha} + \frac{\partial(HvC)}{\partial \beta} + \frac{\partial(\Omega + W_s/H)C}{\partial \sigma}$$
$$D_H\left[\frac{\partial}{\partial \alpha}\left(H\frac{\partial C}{\partial \alpha}\right) + \frac{\partial}{\partial \beta}\left(H\frac{\partial C}{\partial \beta}\right)\right] + (D_V/H)\frac{\partial^2 C}{\partial \sigma^2} \tag{2}$$

The nature of equation (2) requires both the specification of initial and boundary conditions to complete the mathematical model.

Boundary conditions for suspended particles transport

The boundary conditions which were used for particles transport in the South Biscayne Bay are zero convective and diffusive mass flux across the lateral boundaries, zero flux across the free surface and deposition of suspended particles at the bottom surface. Thus, the particles transport boundary conditions in summary are:

At lateral boundaries

$$\frac{\partial C}{\partial \alpha} = 0 \text{ at } y\text{-boundaries}$$

$$\frac{\partial C}{\partial \beta} = 0 \text{ at } x\text{-boundaries}$$

At the free surface

$$-W_s C + \left(\frac{D_V}{H}\right)\frac{\partial C}{\partial \sigma} = 0$$

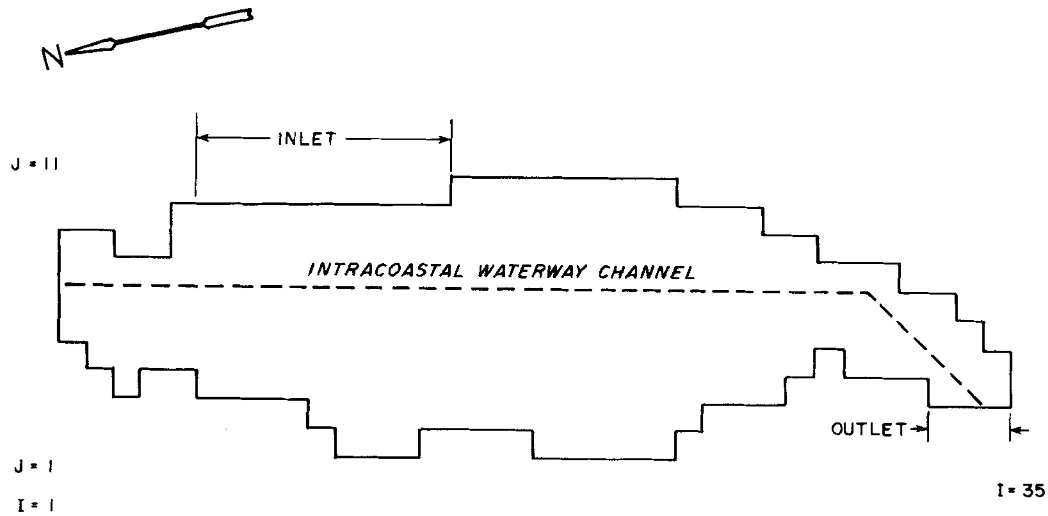

Figure 2. Horizontal grid system for bay in suspended particles transport study

At the bottom surface

$$\left(\frac{D_V}{H}\right)\frac{\partial C}{\partial \sigma} = W_s C(1-A)$$

Where A = probability of suspended particles leaving suspension and depositing on the bottom bed. It represents the rate of mass transfer from suspension to the bed. In these numerical studies two different values for A have been used, namely $A = 0{\cdot}3$ and $A = 0{\cdot}9$.

Initial conditions for particles transport

The numerical study of suspended particles transport for the South Biscayne Bay consisted of specifying an instantaneous line source of unit concentration as shown in Figure 2. That is:

$C(\alpha, \beta, \sigma) = 1,$ along channel (uniform in depth variable, σ)
$C(\alpha, \beta, \sigma) = 0,$ elsewhere

METHOD OF SOLUTION

A finite difference method of solution is used. Figure 3 shows the unstaggered horizontal grid system used in the solution procedure, although meshing techniques are given in Appendix II and III. An explicit forward time method is used for the hydrodynamic model equations with a Dufort–Frankel scheme on the vertical diffusion terms. The other terms have been centrally differenced in space. Although implicit, ADI and other techniques are available for numerical integration, it is noted that for problems of complex boundary geometry and bottom topography, explicit integration in time is suitable.[27] The numerical complexities and iterative solutions associated with implicit schemes often offset the advantages of larger time steps associated with implicit schemes in three-dimensional, free-surface flows. The concentration equation is differenced in a similar explicit manner except that second upwind differencing[28] is used in the horizontal convection

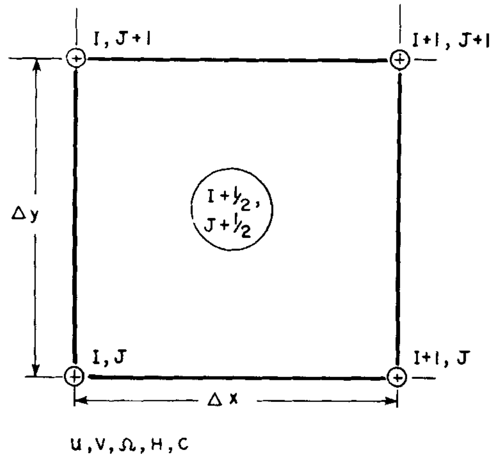

Figure 3. Indexing system in the horizontal plane in unstaggered grid

terms (Appendix II). The coupling the hydrodynamic model to the particle transport model is only in one direction and, therefore, at first the surface heights and current velocities are obtained, followed by concentration calculations. Note that in this study a time step, Δt, of 2 min was used, based upon vertical diffusion as the dominant transport process. Also, owing to the rapid bottom bed deposition, governed mainly by the settling velocity effect, the two models were run simultaneously, instead of holding the hydrodynamic variables constant over a short time interval.[11] The details of the numerical schemes and solution procedure are shown by Sengupta, Lee and Miller.[1]

It was learned that the use of central differencing of the horizontal convection terms in equation (2) resulted in negative concentrations. Lam[29] points out that the central difference approximation will be over-estimating the advective flux in a particular cell so much that it often causes a negative concentration to appear in the neighbouring cell. This problem was circumvented by using the second upwind differencing method. It is important to note that numerical dispersion was not encountered by using second upwind differencing, since particle transport by vertical diffusion and vertical convection, due to settling velocity, were the two dominant transport processes. If this was not the case, flux-corrected transport methods for a convection dominated flow could have been employed.[30] Conservation of mass was ensured at the free surface and at the bottom boundary by using a control volume integral method, thus yielding two additional explicit finite difference equations for the free surface and bottom boundary, respectively (Appendix III).

Numerical stability criteria

The appropriate stability criteria are the Courant–Lewy–Freidrichs condition for surface waves, the convective criteria and the diffusive criteria. These are given for this model study as:

(C.L.F.)

$$\Delta t < \frac{\Delta\alpha}{\sqrt{(gh)}} \quad \text{and} \quad \frac{\Delta\beta}{\sqrt{(gh)}}; \quad \text{where} \quad \sqrt{(gh)} \quad \text{is the phase velocity}$$

Convective (horizontal and vertical)

$$\Delta t < \frac{\Delta\alpha}{u_{\max}} \quad \text{and} \quad \frac{\Delta\beta}{v_{\max}}; \quad \text{and} \quad \Delta t < \frac{H\Delta\sigma}{W_s}$$

Diffusive (horizontal and vertical)

$$\Delta t < \frac{(\Delta\alpha)^2}{2D_{\rm H}} \quad \text{and} \quad \frac{(\Delta\beta)^2}{2D_{\rm H}}; \quad \text{and} \quad \Delta t < \frac{(H\Delta\sigma)^2}{2D_{\rm V}}$$

It should be noted that these criteria are heuristic extensions of Von Neumann stability analysis of the one-dimensional Burgers' equation. The complete three dimensional non-linear governing equations cannot be analysed uniquely for stability. In general, the criteria for the actual three-dimensional system of equations are more restrictive.

For the South Biscayne Bay in this model study, $\Delta\alpha = \Delta\beta = 1{\cdot}6$ km, h ranged from 0·6 m to 4 m, u and v ranged from about 5 cm/s to 50 cm/s (at the inlet), $D_{\rm H} = 10{,}000\ {\rm cm}^2/{\rm s}$, $D_{\rm V} = 0{\cdot}0018\, H^{4/3}\ {\rm cm}^2/{\rm s}$ and $W_{\rm s} = 0{\cdot}02$ cm/s and 0·04 cm/s. Thus, the dominant transport process was, indeed, vertical diffusion. Competing for the next most important transport process were vertical convection with settling velocity $W_{\rm s}$, and surface gravity waves. Horizontal convection and horizontal diffusion were learned to be less important than the vertical transport mechanisms for suspended particles transport.

Therefore, based upon these stability criteria, the numerical diffusion resulting from the second upwind differencing of the horizontal convection terms in the mass transport model (equation (2)), is not of the same order of magnitude as vertical diffusion and vertical convection on the time scale of the integration time step, Δt, of 2 min. Actually, this numerical diffusion could be lumped with the already quite small horizontal diffusion, and not adversely affect the solution. It is important to note that the inertial effects of advection did significantly skew the resulting distributions of suspended particles (Figures 6 and 7), provided that the settling velocity, $W_{\rm s}$, was small ($W_{\rm s} = 0{\cdot}02$ cm/s, not $W_{\rm s} = 0{\cdot}04$ cm/s). Consequently, the sharp initial gradient of sediment particles, was dramatically dispersed by vertical transport mechanisms, rather than by advective fluxes. Hence, the Gibbs' phenomenon due to advection was expected to be negligible. Incidentally, except for the inertial effect of advection upon the concentration profiles (Figure 7), the predicted solution could nearly be obtained by the exact solution of the one-dimensional vertical transport problem of unsteady convection–diffusion. An exponential functional dependence results with a strong dependence on settling velocity.

RESULTS AND DISCUSSION

The concentration equation for suspended particle transport was run coupled to the hydrodynamic model with a time step, Δt, of 2 min. This was done since the overall run time until 90 per cent particle deposition was not long enough to warrant storing hydrodynamic variables on magnetic tape, as was done by Sengupta, Miller and Lee for long-term chemical flushing studies in the South Biscayne Bay. The computer model was run for an instantaneous line source of unit concentration of sediment particles along the y-direction (J-direction in grid system) and uniform in depth (σ-direction). The values of settling velocity, $W_{\rm s}$, and bottom deposition rate, A, were varied to gain physical insight into the governing mechanisms of sediment transport.

Figure 4 illustrates the sediment particle concentration distribution at the surface, $K = 1$, for a J-transect at $I = 13$, so that the effect of the ocean exchange area (inlet) could be studied. The first two cases are for $A = 0{\cdot}9$ and $W_{\rm s} = 0{\cdot}02$ cm/s and $W_{\rm s} = 0{\cdot}04$ cm/s, respectively. Figure 5 illustrates the case for $A = 0{\cdot}3$ and $W_{\rm s} = 0{\cdot}04$ cm/s. The three cases were plotted for a period of one and two hours, respectively. It can be readily seen that doubling the settling velocity, $W_{\rm s}$, strongly affects the distribution of sediment particles in terms of particulate dispersion. However, the affect of tripling the deposition rate, A, is relatively minor upon the shape of the concentration distribution, and the associated mixing effects.

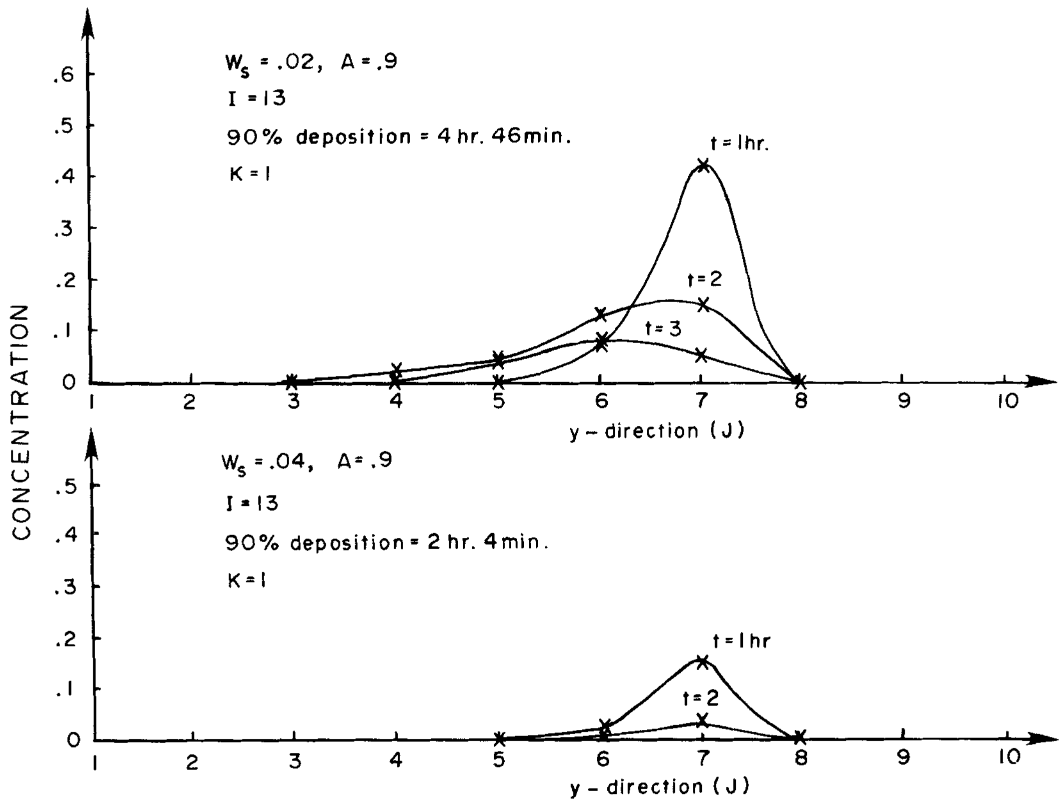

Figure 4. Sediment particle concentration vs. y-direction at surface at $I = 13$

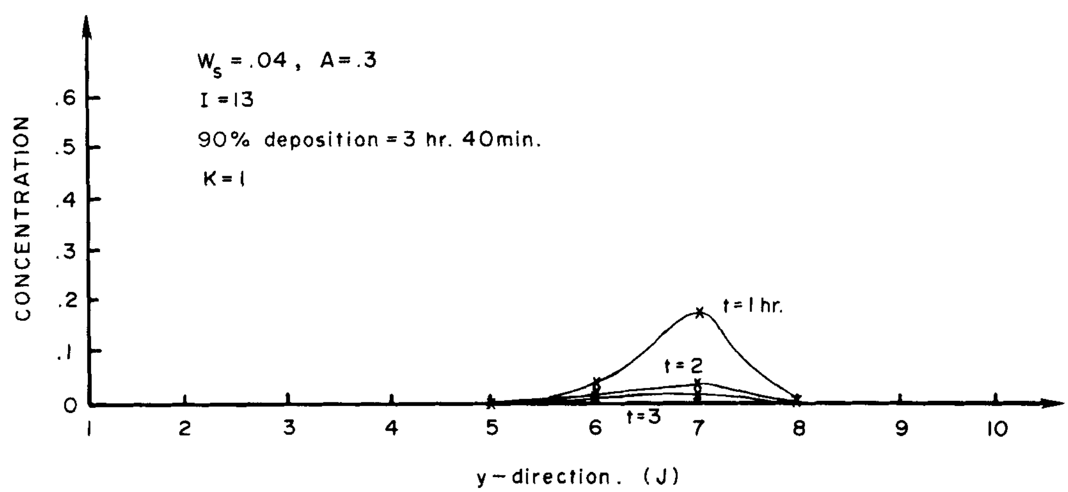

Figure 5. Sediment particle concentration vs. y-direction at surface at $I = 13$

Secondly, it can be seen that the effect of the advection from the incoming tidal current significantly skews the concentration distribution at $I = 13$, which is a J-transect normal to the bay inlet. This advection effect is more greatly demonstrated for the smaller values of settling velocity, where mixing is less dominant, and horizontal inertial effects become prominent.

Note, further, that 90 per cent bottom bed deposition occurred at 4 h, 46 min for $W_s = 0{\cdot}02$ cm/s, $A = 0{\cdot}9$; at 3 h, 40 min for $W_s = 0{\cdot}04$, $A = 0{\cdot}03$ and at 2 h, 4 min for $W_s = 0{\cdot}04$ cm/s, $A = 0{\cdot}9$. Hence, bottom deposition rate, A, strongly affects the amount of sediment particles leaving suspension and accumulating on the bed, but does not appreciably affect the shape of the concentration distribution.

Figure 6 illustrates sediment particle concentration vertical profiles for $I = 13$, $J = 7$, near the inlet; and Figure 7 at $I = 21$, $J = 7$ where the flow field is uniform and aligned in the y-direction (J-direction). This case is for $W_s = 0{\cdot}02$ cm/s and $A = 0{\cdot}9$. As can be seen, the vertical profiles fell off rapidly with increasing time, and the influence of advection is again clearly indicated. That is the faster advection currents at $I = 13$, $J = 7$ strongly convected the initially uniform concentration profile, compared to the smaller advection currents at $I = 21$, $J = 7$.

Thus, the effects of advection, settling velocity and bottom deposition rate have been clearly identified for the case of ideal gravitational settling in a three-dimensional, free-surface flow field. Again, it is useful to note that bottom bed scour is ignored in the mass transport model.

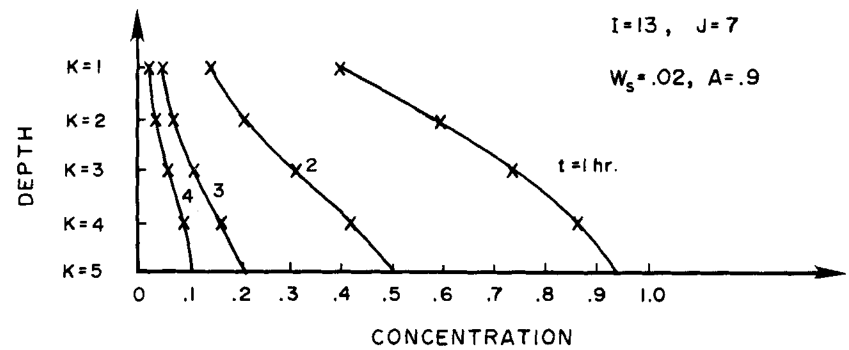

Figure 6. Vertical sediment particle profiles at $I = 13$, $J = 7$

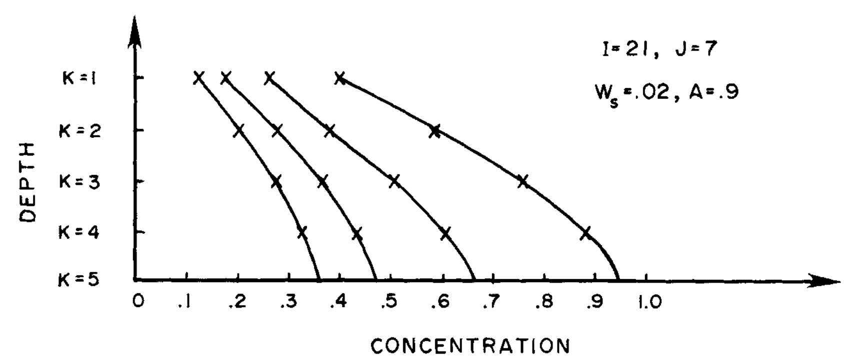

Figure 7. Vertical sediment particle profiles at $I = 21, J = 7$

CONCLUSIONS

The basic suspended particles transport processes, with associated boundary conditions, have been modelled. General features of the suspended sediment particles transport have been evaluated qualitatively, and the resulting behaviour and dominant physical process determined. The most recent hydrodynamic model used by other researchers is that of Sheng.[5] However, this model relaxes Sheng's 'rigid-lid' approximation, by actually treating the bay's free surface behaviour. In order to treat, properly, the tide level variations in a shallow bay and the short time scales for tidal current reversal, a free surface is required. Thus, the effects of variable tidal level for bay system suspended particles transport has been accomplished by employing a three-dimensional, time-dependent free-surface model.

By varying the values of particle settling velocity and bottom deposition rate, physical insight was gained with regard to the governing mechanisms of suspended particles transport. It has been learned that the resulting distribution of suspended sediment particles is much more strongly affected by varying settling velocity than by varying bottom deposition rate.

The effects of ideal gravitational particle settling with variable settling velocity have not been discussed by the above researchers. However, Sheng[5] and Jobson[8] have reported the results of using variable bottom deposition rate in their studies. This investigation, *vis-à-vis* a thorough comparison with the state-of-the-art of research in sediment particles transport is, therefore, the most realistic with regard to modelling the hydrodynamic field, and as well as including variable settling velocity and variable bed deposition rate in the mass transport model.

Further research into other physical processes of sediment particles transport, such as hindered particles settling, flocculation, and bed scour (or ciscous turbulent entrainment), would be the next logical step in properly modelling sediment particles transport in geophysical flows. However, realistic descriptions of these complicated physical processes requires much more experimental research. Present descriptions are empirical in nature,[17,18] and relative interaction between these processes has not, as yet, been determined. Thus, until a better experimental base exists, introduction of these physics is a task not worth pursuing. The above mentioned researchers also limited their investigations to ideal gravitational particle settling, since in actual flows the databases for sediment particles transport are virtually non-existent.

This model can be directly applied to surface water dispersion of particulates in a tidal bay. However, the mathematical model is general enough to be applied, as well, to particulates dispersion in a variety of water bodies. There is a size (diameter) limitation on the suspended particulates in order to properly employ the present numerical model.

The effects of dredging and landfill operations can be studied by using this particulate dispersion model. The example presented in this paper gives an application to a dredging operation, whereby an instantaneous line source of particulate matter is dispersed in a naturally occurring three-dimensional flow field, including the intrinsic particle effect of settling velocity, and estimates of bottom bed deposition.

APPENDIX I—NOMENCLATURE

A = Bottom bed deposition probability
C = Concentration of suspended sediment particle
D_H = Eddy mass diffusivity in horizontal direction
D_V = Eddy mass diffusivity in vertical direction
g = Acceleration due to gravity
h = Depth relative to the mean water level
H = Depth contour relative to the free surface, $h + \eta$

I = Grid index in x-direction, or α-direction
J = Grid index in y-direction, or β-direction
K = Grid index in z-direction, or σ-direction
t = Time
u = Velocity component in x-direction
v = Velocity component in y-direction
w = Velocity component in z-direction
U = α-velocity component in (I, J, K)
V = β-velocity component in (I, J, K)
W_s = Suspended particle settling velocity
x = Horizontal co-ordinate
y = Horizontal co-ordinate
z = Vertical position relative to the mean water level
Z = Vertical position relative to the free-surface, $z + \eta$
α = Horizontal co-ordinate in stretched system, x
β = Horizontal co-ordinate in stretched system, y
σ = Vertical co-ordinate in stretched system, Z/H
Ω = Transformed (or equivalent) vertical velocity
η = Free-surface elevation above mean water level

Subscripts

H = Horizontal quantity
o = Quantity at inlet (ocean-exchange area)
s = Quantity at free surface
V = Vertical quantity

APPENDIX II—SECOND UPWIND DIFFERENCING OF HORIZONTAL CONVECTION TERMS IN THE MASS TRANSPORT EQUATION

It was learned in the numerical studies that the use of central differencing of the convective derivatives in equation (2) resulted in negative species concentrations. Lam[29] points out that the central difference approximation will be overestimating the advective flux so much that it often causes a negative concentration to appear in the neighbouring cell. To circumvent this problem, the so-called second upwind differencing method, or donor cell method introduced by Gentry, Martin and Daly[28] was used in these numerical studies.

Some sort of average interface velocities on each side of the grid cell are defined, and, then, the signs of these velocities determine, by upwind differencing, which value of concentration, C, to use. Following Roache,[27] in one-dimensional notation,

$$\frac{\Delta C_I}{\Delta t} = -\frac{U_R C_R - U_L C_L}{\Delta x} \tag{3}$$

Approximates

$$\frac{\partial C}{\partial t} = -\frac{\partial (uC)}{\partial x}$$

where

$$U_R = \tfrac{1}{2}(U_{I+1} + U_I)$$
$$U_L = \tfrac{1}{2}(U_I + U_{I-1})$$

and

$$C_R = C_I \quad \text{for} \quad U_R > 0; \quad C_R = C_{I+1} \quad \text{for} \quad U_R < 0$$
$$C_L = C_{I-1} \quad \text{for} \quad U_L > 0; \quad C_L = C_I \quad \text{for} \quad U_L < 0$$

For $U_R > 0$, $U_L > 0$:

$$\frac{\Delta C_I}{\Delta t} = -\left(\frac{U_R C_I - U_L C_{I-1}}{\Delta x}\right) \tag{4}$$

For $U_R < 0$, $U_L < 0$:

$$\frac{\Delta C_I}{\Delta t} = -\left(\frac{U_R C_{I+1} - U_L C_I}{\Delta x}\right) \tag{5}$$

For $U_R > 0$, $U_L < 0$:

$$\frac{\Delta C_I}{\Delta t} = -\left(\frac{U_R C_I - U_L C_I}{\Delta x}\right) \tag{6}$$

For $U_R < 0$, $U_L > 0$:

$$\frac{\Delta C_I}{\Delta t} = -\left(\frac{U_R C_{I+1} - U_I C_{I-1}}{\Delta x}\right) \tag{7}$$

Now, for equation (2), we have the following form for the horizontal convection terms,

$$\frac{\partial(HuC)}{\partial\alpha} \quad \text{and} \quad \frac{\partial(HvC)}{\partial\beta}$$

Thus, by merely replacing U_R and U_L with $(HU)_R$ and $(HU)_L$, $(HV)_R$ and $(HV)_L$, Equations (4)–(7) can be readily applied, where:

$$(HU)_R = \tfrac{1}{2}(H_{I,J} + H_{I+1,J}) \times \tfrac{1}{2}(U_{I,J,K} + U_{I+1,J,K})$$
$$(HU)_L = \tfrac{1}{2}(H_{I,J} + H_{I-1,J}) \times \tfrac{1}{2}(U_{I,J,K} + U_{I-1,J,K})$$
$$(HV)_R = \tfrac{1}{2}(H_{I,J} + H_{I,J+1}) \times \tfrac{1}{2}(V_{I,J,K} + V_{I,J+1,K})$$
$$(HV)_L = \tfrac{1}{2}(H_{I,J} + H_{I,J-1}) \times \tfrac{1}{2}(V_{I,J,K} + V_{I,J-1,K})$$

Note that the method is both conservative and transportive, and is more accurate than first upwind differencing. The South Biscayne Bay is dominated by vertical diffusion,[1] and, therefore, numerical dispersion, which would result from upwind differencing in a convection dominated flow,[30] was not encountered in these studies.

APPENDIX III—CONTROL VOLUME FORMULATION OF BOUNDARY FINITE DIFFERENCE EQUATIONS

A conservation of mass control volume formulation is used to ensure against significant mass leakage in the numerical model at the free surface and bottom boundaries. Merely substituting the appropriate boundary conditions into the interior explicit finite difference equation does not conserve mass. Hence, two additional finite difference equations for the free surface and bottom boundaries have been derived. Then, upon substitution of the free surface and bottom boundary conditions into these equations, mass is conserved.

Equation (2) is rearranged with the unsteady term on the left as follows:

$$\frac{\partial(HC)}{\partial t} = -\frac{\partial(HuC)}{\partial\alpha} - \frac{\partial(HvC)}{\partial\beta} - H\frac{\partial(\Omega' C)}{\partial\sigma}$$

$$+D_{\mathrm{H}}\left(\frac{\partial}{\partial\alpha}\left(H\frac{\partial C}{\partial\alpha}\right)+\frac{\partial}{\partial\beta}\left(H\frac{\partial C}{\partial\beta}\right)\right)$$
$$+\left(\frac{D_{\mathrm{V}}}{H}\right)\frac{\partial^2 C}{\partial\sigma^2} \tag{8}$$

where

$$\Omega' = \Omega + W_s/H$$

Then equation (8) is integrated over the volume of a half-cell either at the free surface or the bottom boundary, and integration over Δt is also performed. The volume of this half-cell $= H/2\Delta\alpha\Delta\beta\Delta\sigma$. Upon integrating equation (8) over $H/2\Delta\alpha\Delta\beta\Delta\sigma$ and over Δt, the integral of the unsteady term becomes for the free surface:

$$\int_0^{\Delta t}\int_{I-1/2}^{I+1/2}\int_{J-1/2}^{J+1/2}\int_K^{K+1/2}\frac{\partial(HC)}{\partial t}\frac{H}{2}\mathrm{d}\alpha\mathrm{d}\beta\mathrm{d}\sigma\mathrm{d}t$$
$$=\int_\alpha\int_\beta\int_\sigma (H^{n+1}C^{n+1}-H^nC^n)\frac{H}{2}\mathrm{d}\alpha\mathrm{d}\beta\mathrm{d}\sigma$$

By application of the mean value theorem a volume averaged concentration in the half-cell is obtained:

$$H_{I,J}C_{I,J,K}=\left\{\frac{1}{\Delta\alpha\Delta\beta\Delta\sigma H_{I/2,J/2}}\right\}\int_{I-1/2}^{I+1/2}\int_{J-1/2}^{J+1/2}\int_K^{K+1/2}(HC)H\mathrm{d}\alpha\mathrm{d}\beta\mathrm{d}\sigma$$

The surface averages are defined for the convective and diffusive fluxes crossing the cell boundaries as follows; in the α-direction:

$$\Delta t\int_\beta\int_\sigma\{(HuC)_{I+1/2}-(HuC)_{I-1/2}\}H_{I,J}\,\mathrm{d}\beta\mathrm{d}\sigma$$
$$=\Delta t\{(HuC)_{I+1/2}-(HuC)_{I-1/2}\}\underbrace{\frac{H\Delta\beta\Delta\sigma}{2}}_{\text{Surface area}}$$

and, similarly in the β- and σ-directions, for convection. For diffusion in the α-direction,

$$\Delta t\int_\beta\int_\sigma\left(D_{\mathrm{H}}H\frac{\partial C}{\partial\alpha}\right)_{I-1/2}^{I+1/2}H\mathrm{d}\beta\mathrm{d}\sigma=D_{\mathrm{H}}\Delta t\left(H\frac{\partial C}{\partial\alpha}\right)_{I-1/2}^{I+1/2}\frac{H}{2}\Delta\beta\Delta\sigma$$

and, similarly in the β and σ-directions, for diffusion. Finally, the free-surface boundary condition is substituted into the newly derived boundary finite difference equation:

$$W_sC_K^n=\frac{D_{\mathrm{V}}}{H}\frac{\partial C}{\partial\sigma}\bigg|_K^{n,n+1,n-1}\quad\text{at the free-surface}$$

where

$$\frac{\partial C}{\partial\sigma}\bigg|_{K+1/2}^{n,n+1,n-1}=\frac{C_{K+1}^n-(C_K^{n+1}+C_K^{n-1})/2}{\Delta\sigma}$$

and

$$C_{K+1/2}\simeq(C_K+C_{K+1})/2$$

Similarly, the bottom boundary condition can be obtained by integrating over the bottom half-cell by replacing the limits of integration over $\mathrm{d}\sigma$ with $K-1/2$ for K and K for $K+1/2$.

The bottom boundary condition used is given by:

$$\left.\frac{D_V}{H}\frac{\partial C}{\partial \sigma}\right|_K^{n,n+1,n-1} = W_s C_K^n (1 - A)$$

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