Feasibility of Coupled Three-Dimensional Hydrodynamic and Water Quality Modeling of the Peconic Bays System

INTERIM REPORT #1

Prepared for:

Peconic Estuary Program
County of Suffolk
Department of Health Services
Evans K. Griffing County Center
Riverhead, NY 11901-3397

Prepared by:

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April 10, 1996

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April 10, 1996

Vito Minei, P.E., Program Manager
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Evans K. Griffing County Center
Riverhead, NY 11901-3397

Subject: *Peconic Estuary Program, Interim Report #1*

Dear Vito ~~Mr. M~~inei:

We are enclosing three (3) copies of the report *Feasibility of Coupled Three-Dimensional Hydrodynamic and Water Quality Modeling of the Peconic Bays System* in fulfillment of Task #1 of the Scope of Services for our Peconic Estuary Program Surface Water Quality Modeling contract.

This report expands on the original scope of work by including a review and comparison of available 3-dimensional hydrodynamic and water quality models in addition to providing background on recent hydrodynamic work in the Peconic system. The primary conclusion is that a 3-D hydrodynamic and water quality simulation of the Peconic Estuary is feasible using a relatively low-cost Pentium Pro desktop computer.

We believe the use of a 3-D model will provide the Peconic Estuary Program with a substantially more useful scientific tool than the DYNHYD/WASP link-node model developed under the BTCAMP study. For example, the 3-D model will be able to answer questions regarding the effects of subtidal sea-level oscillations (i.e., subtidal volume fluxes) as well as the localized impacts of Shinnecock Canal with much more credibility than is possible with the link-node model.

If you have any comments or questions on the enclosed report, or if you need additional copies to distribute to members of the Model Evaluation Group, please let me know.

Sincerely,

M.R. Mot

Michael R. Morton, P.E.
Principal Engineer

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February 1996

Report JHM-TTI-96-1

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February 28, 1995

Mr. M. R. Morton, P.E.
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Dear Mr. Morton:

Please find attached a report, *Feasibility of Coupled Three-Dimensional Hydrodynamic and Water Quality Modeling of the Peconic Bay System*. This document goes beyond the original scope of work, which was a review of three-dimensional hydrodynamic models appropriate for the Peconic Bays system, to also estimate the feasibility of coupled three-dimensional hydrodynamic and water quality modeling primarily from the point of view of computational performance on desktop computer systems. The primary judgment of feasibility was the criteria of being able to make seasonal to annual time scale simulations using 500 meter to one kilometer horizontal grid resolution with run times on the order of days. Estimates, documented in the report, indicate that a coupled three-dimensional hydrodynamic model and WASP5 equivalent water quality model would achieve the set criteria with run times on the order of 25 to 50 hours for one year simulations on Pentium Pro desktop systems which have recently become available.

Other important issues addressed in this document include: open boundary conditions consistent with the larger scale Long Island Sound hydrodynamic and water quality models; representation of small bays connected to the main bay system by short, narrow inlets; and the representation of Shinnecock Bay, Shinnecock Inlet and the Shinnecock Canal. A number of alternatives are presented for the location of boundaries. A modification of the flow control structure formulation in the EFDC model is shown to provide an appropriate representation of flow and mass transport through narrow

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1. Introduction

The purpose of this report is to review three-dimensional hydrodynamic models appropriate for modeling the Peconic Bays estuarine system and to investigate the feasibility of coupled three-dimensional hydrodynamic and water quality modeling of the system. The Peconic Bays, Figure 1, are a system of shallow interconnected bays situated between the north and south forks of Eastern Long Island. Great Peconic and Little Peconic Bays comprise the largest bays of the system with Noyack and Flanders Bay being among the most significant of the smaller components. The system connects to Gardiners Bay by two passages around Shelter Island. Gardiners Bay adjoins both Long Island Sound and Block Island Sound. The shoreline of the Peconic Bays system a characterized by numerous narrow inlets connecting small bays, having surface areas typically on the order of 10 square kilometers or less.

The water surface area of the Peconic Bays systems is approximately 218 square kilometers and the average depth is approximately 8 meters. Point sources of fresh water inflow into the system account for an approximate annual mean inflow of only 1 cubic meter per second, with the remaining fresh water inflow being due to nonpoint source runoff and groundwater inflows. Tides in the system are primarily durinal with maximum ranges being on the order of 85 centimeters. Tidal currents may reach 1 meter per second in the vicinity of headlands. The low fresh water inflow, combined with moderate tidal flow and local and nonlocal wind driven flows, results in the system being classified as having a vertically mixed salinity regime.

For subsequent discussions, it is useful to define an extended Eastern Long Island bay system that includes the Peconic system, Gardiners and Napeague Bays, and the portion of Block Island Sound southwest of the line between Plum Island and Montauk Point, since this line defines of natural geographic boundary. It is also desirable to include Shinnecock Bay, on the southern shore of Long Island, in this system, since Shinnecock Bay connects with Great Peconic Bay by the Shinnecock Canal and connects with the Atlantic Ocean through Shinnecock Inlet.

Previous modeling studies of the Peconic Bays system include both hydrodynamic (Gomez-Reyes, 1986&1989; Schmalz, 1992&1994; Sun, 1992; Wei, 1992), and combined hydrodynamic and water

2. Hydrodynamic Modeling Requirements for the Peconic Bays System

The general hydrodynamic modeling requirements for the Peconic Bays System may be grouped into four categories including: the hydrodynamic model's representation of physical processes; its flexibility with respect to diverse applications including linking to water quality models; its ease of use including preprocessing and post processing features; and the cost of the model's development or acquisition, maintenance, support and operation. Of these model requirements, the representation of physical processes is obviously the most important, but the other categories should be considered particularly when comparing models which have equivalent process representations.

To aid in the following discussion, it is useful to introduce some generic hydrodynamic modeling terminology. In referring to the horizontal grid employed by finite difference, finite volume, and finite element numerical models, the term 'cell' will denote the enclosed horizontal boundary over which discrete conservation of volume is enforced. Most contemporary finite difference and finite volume free surface flow models employ grids which bound computational cells with the water surface elevation and the concentration of dissolved and suspended material represented as a cell average quantity located at the cell center. Horizontal flow occurs across the cell faces which are also the grid boundaries. Many finite difference and finite volume models, referred to as staggered grid models, locate the velocity and volume flux variables on, and normal to, the cell faces, while some finite volume models locate the velocity variables at the cell centers and calculate the volume flux across the cell faces using averaging schemes of varying sophistication, Figure 2. Grid lines bounding cell faces in finite difference and finite volume models are constant coordinate surfaces of Cartesian, curvilinear-orthogonal, or general curvilinear coordinate systems. For finite element models, the horizontal element mesh defines the horizontal computational cells which are coincident with the elements. For finite element models, the surface elevation may be represented at the element or cell center or at the vertices of the cell, which are referred to as nodes, while the horizontal velocity vectors are located at the nodes with volume flux across the cell faces determined by interpolation or integration between bounding nodes, Figure 2. Finite element models employ local coordinate systems within each element, with the local coordinate system external unmodeled region are necessary. For tidal flow, the tide wave propagates inward and outward across the open boundaries. Atmospheric forcings can be split into two classes, the first being local forcing by surface wind stress action inside the model domain. The second component of the atmospheric forcing, termed nonlocal forcing, arises due to the action of wind stress and atmospheric pressure gradients outside the model domain. The nonlocal atmospheric forcing is manifest by variations in sea level along the model domain's open boundaries. The simplest specification of tidal and nonlocal atmospheric forcings on the open boundary is the specification of the water surface elevation or instantaneous sea level. The primary problem with the specification of the elevation only boundary condition is that waves generated in the model domain, either by local forcing or by reflection of incoming waves associated with inward tidal propagation and nonlocal atmospheric forcings, cannot freely pass out of the model domain across the open boundary (Bennett, 1976; Bennett and McIntosh, 1983). An alternative to the specification of only the water surface elevation on the open boundary is the use of radiation or radiation-separation boundary conditions (Hamrick, 1996a). The radiation and radiation-separation boundary conditions are based on the inward, boundary normal, wave propagation characteristic:

$$g\zeta - \sqrt{gH}\mathbf{n} \bullet \mathbf{u} = R \tag{1}$$

where ζ is the water surface elevation, H is the depth, $\mathbf{u}$ is the barotropic or depth averaged velocity vector, and $\mathbf{n}$ is the unit vector outward normal to the boundary. The radiation-separation condition requires the specification of the incoming wave characteristic, R, with the out going characteristic remaining a free quantity. If the incoming characteristic R is correctly specified, the incoming wave is properly described and outward propagating waves pass across the boundary without reflection back into the model domain. The major difficulty with the specification of the relation (1) as opposed to specification of only the water surface elevation, ζ , is knowledge of the normal velocity component. A number of inverse or identification schemes (Bennett and McIntosh, 1983; Hamrick, 1996b) have been developed to determine the boundary condition specified by equation (1) during the calibration of a hydrodynamic model such that a best fit between model predictions and observed water surface elevations inside the model domain, is achieved. Hamrick (1996b) indicated that the identification scheme becomes more effective as the alignment of the where *B*, *h*, and *L* are the width, depth, and length of the inlet, and *Q* is the maximum flow rate through the inlet. When the inlet length is significantly smaller than the horizontal grid spacing used in the larger open regions of the model domain, the inlet will control the model's time step. Another problem exists in that the width of model cells on the two extremities of the inlet should be on the order of the inlet width, thus the potential of further time set reduction exist since the time step in the open regions is constrained by:

$$\Delta t \le \left(\frac{u}{dx} + \frac{v}{dy} \right)^{-1} \tag{3}$$

where *u* and *v* are the horizontal velocities in the *x* and *y* directions and *dx* and *dy* are the horizontal dimensions of the corresponding grid cell. For an inlet aligned in the *y* direction, the grid spacing *dx* of cells north and south of the inlets should be on the order of *B*, the inlet width. An example of an inlet controlling the grid spacing over a large area of a model domain is given by Jones, *et al.* (1994). Representation of the Shinnecock Inlet also poses a similar problem in terms of the cell width constraint in Shinnecock Bay. Although mush longer than the typical tidal inlets in the bay system, the direct representation of the narrow Shinnecock Canal will likely constrain grid cell dimensions in Shinnecock and Great Peconic Bays and in turn constrain the time step as indicated by equation (3).

There are a number of alternatives to direct representation of tidal inlets and the Shinnecock Canal in a hydrodynamic and water quality model of the Eastern Long Island Bays system. The two alternatives, a subgrid scale channel representation and a flow control structure representation, can be incorporated into any multidimensional hydrodynamic model and have been incorporated into the EFDC model as documented by Hamrick (1994b). The subgrid scale channel model was developed to represent deep narrow channels passing through a two-dimensional horizontal domain having grid cell spacings an order of magnitude or more larger than the width of the channels. In this formulation, the two-dimensional depth averaged hydrodynamic momentum equations and the one-dimensional cross section averaged hydrodynamic momentum equations are solved independently on the larger scale horizontal grid and in the channel network under the constraint that the water surface elevation in a channel segment passing through a two-dimensional cell be identical to the water surface elevation in that software either internal or external to the model code. External preprocessing is generally preferable in that a large per cent of the input data will not change during the course of model calibration and validation for a particular application. A typical preprocessor software package should include grid generation and bathymetric data processing and generate model input files which describe the geometry and bathymetry of the region being modeled. A flexible model should also include combinations of internal and external postprocessing, allowing model results to be readily interpreted in both numerical and graphical form. Typical model output used for both graphical and numerical interpretation include time series at selected spatial locations and two and three dimensional spatial snapshots of model variables at selected time intervals. Direct or postprocessed model output for graphic and visualization interpretation should be in a compact format general enough for use with a number of graphics and visualization software packages rather than custom formatted for the software package chosen by the model developer.

Closely related to a model's ease of use and flexibility, is the availability of documentation describing both the model's theory and use. In this regard a generic and optional application specific model user's manual consistent with the version of the model source code is essential. A final issue relates to model acquisition. Few organizations are capable of funding the development of a new hydrodynamic and transport modeling package, the cost of which is typically in the hundreds of thousands of dollars. The model choice is then between public domain and proprietary modeling packages, noting that a number of models have both public and private versions. In this regard a public domain model package having a reasonably long record of applications and support by either the model developer, the developing organization or a third party would likely be the most economical choice.

(Hamrick, 1992a,b, 1996a,b) and the TRIMM model (Casulli and Cheng, 1992). The CH3D-WES (curvilinear hydrodynamics in three dimensions) model is a public domain model developed and supported by the U. S. Army Engineers Waterway Experiment Station. The ECOM (estuary and coastal ocean model) or POM (Princeton ocean model), also widely known as the Blumberg-Mellor model, exist in both public and private versions. The generic public version was originally developed with support from a number of federal agencies at Princeton University and is available by FTP on the INTERNET. A proprietary version of ECOM is maintained and supported by HydroQual, Inc. The public domain EFDC (environmental fluid dynamics code) model was originally developed at the Virginia Institute of Marine Sciences of the College of William and Mary, and is available from VIMS. An enhanced public domain version of the EFDC model as available from Tetra Tech, Inc., which also provides support from the model developer. The TRIMM (tidal, residual, and intratidal mudflats models) model is a public domain model developed and supported by the U. S. Geological Survey. The two most widely used three-dmensional finite element models to are the RMA10 and ADCIRC models. The RMA10 model (King, *et al.*, 1994) was developed by Resource Management Associates and the University of California at Davis. The RAM10 model has been applied to a number of estuaries including a two-dimensional simulation of San Francisco Bay (DeGeorge and King, 1994). The public domain version of RMA10 was funded by the U. S. Army Corps of Engineers, Waterway Experiment Station which also distributes the model. The ADCIRC (advanced circulation) model (Westerink, *et al.*, 1992) was developed at the Universities of Notre Dame and North Carolina, with funding primarily from the U. S. Army Corps of Engineers, Waterway Experiment Station. The ADCIRC model has been applied primarily for large scale coastal tidal and storm surge simulation and no three-dimensional estuarine or bay applications have been reported to date.

The CH3D-WES model employs a general curvilinear grid in the horizontal and has both Cartesian and stretched vertical grid versions. The model is based on extensive modifications to the earlier CH3D developed by Sheng (1990). Major applications of CH3D-WES include: Chesapeake Bay (Johnson, *et al.*, 1993), Delaware Bay (Kim, *et al.*, 1994), Galveston Bay (Berger, *et al.*, 1994), New York Bight (Kim *et al.*, 1992), and New York Bight with Long Island Sound (Vemulakonda and Scheffner, 1994). The estuarine applications, Chesapeake, Delaware and Galveston Bays, utilized the Cartesian

Feature/ Model	CH3D-WES	ECOM/POM	EFDC	TRIM
Horizontal Grid	general curvilinear	orthogonal curvilinear	orthogonal curvilinear	Cartesian
Vertical Grid	Cartesian or stretched	stretched	stretched	Cartesian
Temporal Integration (flow solution)	explicit advection implicit propagation implicit vertical diff	explicit advection explicit propagation implicit vertical diff	explicit advection implicit propagation implicit vertical diff	explicit advection implicit propagation implicit vertical diff
Temporal Integration (transport solution)	explicit advection implicit vertical diff	explicit advection implicit vertical diff	explicit advection implicit vertical diff	explicit advection implicit vertical diff
Advective Transport Scheme	first order upwind or QUICKEST	centered in time and space	first order upwind or MPDATA	Euler-Lagrange
Transported Scalar Fields	salinity temperature	salinity temperature	salinity temperature sediment	salinity
Turbulence Model	two equation k-ε	two equation q-l	two equation q-l	enhanced mixing length
External Water Quality Models	CE-QUAL-ICM	RCA	WASP5 RCA	none
Internal Water Quality Models	none	none	CE-QUAL-ICM and WASP5 equivalents	none

Table 1. Comparison of Finite Difference Hydrodynamic Models

level implementations. Although the two time level variant is more memory efficient, two time level schemes are subject to rotational instabilities which must be damped by slight enhancements to physical friction. The three-time level variants are not subject two rotational instabilities. The centered in time and space momentum advection scheme used in ECOM often requires horizontal diffusion to reduce spatial noise in the solution fields. [All four models provide for dynamically active transport of salinity and temperature. The * computational representation of advective transport of salinity and temperature, as well as water quality constituents, is generally more critical than the representation of momentum advection.] The CH3D-WES and EFDC models use simple first order upwind difference momentum advection, while using higher order upwind schemes such as QUICKEST and MPDATA for salinity and temperature advection. The Euler-Lagrange scheme used for salinity advection in TRIMM is regarded as computationally efficient, but does not guarantee conservation of salt, which is guaranteed by the schemes used in the other models. [Hydrodynamic models used to drive water quality models must have accurate temperature prediction capabilities due to the sensitivity of water quality processes on ambient temperature. Temperature prediction involves representation of solar heating and atmospheric heat exchange in addition to physical transport.] The CH3D-WES model uses an equilibrium temperature approach for heating and exchange, with most of the computation performed externally in the computation of the equilibrium temperature. The ECOM and EFDC models use the NOAA Geophysical Fluid Dynamics Laboratory's thermal exchange model (Rosati and Miyakoda, 1988), with EFDC also having the equilibrium temperature formulation incorporated as an option. [The TRIMM model does not currently include temperature simulation.] *

[A turbulence closure model is essential to represent vertical mixing * of exchange in density stratified environmental flows. The ECOM and EFDC models use the extended Mellor-Yamada turbulence model (Mellor and Yamada, 1982; Galperin et al., 1988).] The Mellor-Yamada model is based on transport equations for the turbulence intensity and the product of the turbulence intensity and the turbulence length scale, and is referred to as a two equation or second moment closure model. The MY model also includes analytically determined stability functions which account for reduced and enhanced vertical mixing associated with stable and unstable vertical stratification. The CH3D-WES model originally included an algebraic equilibrium turbulence model which was essentially a grid described by Jones et al. (1994) on three different computer systems, a Power Macintosh 7100/66, a Hewlett Packard 735/99 and a Cray C90. These systems represent a range of computing resources with the low end Macintosh system being comparable to a 90 MHZ Pentium system. The Hewlett Packard workstation represents what was considered to be at the high end of workstation performance in 1994. For model runs on each platform, the two codes were compiled using identical optimized complier options. Three simulation were conducted on the Cray C90 systems using respectively one, two and three central processing units with automatic code parallelization compiler options used for generating codes executed on multiple CPUs. Performance results across the three computing platforms were remarkably consistent with the EFDC code executing simulations of identical duration approximately 1.85 times faster than the public domain version of ECOM. To estimate the performance of the EFDC hydrodynamic and water quality models relative to CH3D-WES and CE-QUAL-ICM, results from an EFDC simulation of Chesapeake Bay were compared with reported CH3D-WES and CE-QUAL-ICM results. The built in water quality model in EFDC (Park, *et al.*, 1995) is based on process formulations in CE-QUAL-ICM (Cerco and Cole, 1993) and is considered functionally equivalent. Since the models were executed on different grids and Cray supercomputers, a number of conservative scaling factors were used to arrive at performance measures in units of CPU seconds per cell per year of simulation. For the hydrodynamics only comparison EFDC was estimated to be approximately 12.5 times faster than CH3D-WES. [For combined hydrodynamic and water quality simulations, EFDC was estimated to be 9.5 times faster than CH3D-WES * linked with CE-QUAL-ICM. Given the across platform consistency of the EFDC and ECOM benchmarks, it would be reasonable to expect these performance estimates to also be valid for workstations and high end PC and Macintosh systems.]

1987). A number of exceptions as to the inclusion of horizontal diffusion-like mixing in the transport equation (4) should be noted. In deriving a depth integrated or averaged two-dimensional transport equation from equation (4), depth averaged, non-zero correlations of unresolved horizontal advective fluxes of the from ($u'c'$) and ($v'c'$) arise, where the primes denote vertically varying velocity and concentration deviations from corresponding depth averaged values. These correlations result in a horizontal mass transport process known as shear flow dispersion (Fischer, *et al.*, 1979) and they can be represented in a horizontal gradient flux form as the product of a directionally dependent effective horizontal diffusivity, more appropriately referred to as a shear flow dispersion coefficient. For flow in two horizontal dimensions, the dispersion coefficient is formally a second order four component tensor.

Given the advective transport field and the appropriate diffusion and dispersion transport parameters from the hydrodynamic model simulation, a major concern is selection of a numerical solution scheme for the transport and transformation equation. Numerical schemes for solving transport equations with reactions should be mass conserving and positive definite (Smolarkiewicz and Clark, 1986). A mass conserving scheme is one which is applied to the conservative form of the transport equation (equation 4 is in conservative form) and results in a discrete numerical form which reduces to the discrete numerical form of the continuity equation when diffusion, dispersion, and reaction terms are eliminated from the transport equation and the scalar variable is set to unity over space and time. Such a discrete numerical scheme guarantees that the conservation of scalar mass is consistent with the conservation of volume imposed by the discrete continuity equation.

A positive definite scheme is one in which the sign of a positive scalar variable is preserved, or in other words negative concentrations do not arise as an artifact of the numerical solution scheme. The classic example of a positive definite scheme is the donor cell upwind difference scheme applied to the transport equation written in conservative form. An example of a scheme which is not positive definite is the central difference advection scheme, even when applied in conservative form. Most water quality models utilize positive definite schemes, the most common being the donor cell upwind difference scheme used in the WASP5 model (Ambrose, et al., 1993). Unfortunately, the donor cell scheme introduces artificial or numerical diffusion into the solution of the however in most practical applications one or two anti-diffusive corrections is sufficient. A single anti-diffusion correction is sufficient to make the scheme second-order accurate in space and time. The stability criteria for an explicit implementation of the MPDATA scheme is identical that for the standard donor cell scheme.

A final consideration in selecting numerical schemes for the transport and transformation equation is the treatment of reactive source and sink terms. Most schemes use two sub-steps for the advancement of the solution from the old to the new time level, with physical transport being evaluated in one sub-step and reactive source and sink terms being evaluated in a the second sub-step. The danger in such schemes is that even though the physical transport scheme may be positive definite, the reactive sub-step will not necessarily be positive definite. Smolarkiewicz and Margolin (1993) showed that such schemes are also only first-order accurate, even when a sophisticated high order numerical scheme is used for the physical transport sub-step. Smolarkiewicz and Margolin then proceeded to show that second order accuracy in the numerical solution of the transport and transformation equation can only be achieved through systematic and consistent spatial and temporal discrete representations of the advection, diffusion and reaction terms. The scheme they proposed is fractional step scheme involving first the calculation of a preliminary mid-time step concentration from the old time level concentration using an explicit diffusion and reaction half step. The preliminary mid-time step concentration field is then advected a full time step by the explicit MPDATA scheme to obtain a preliminary new time level concentration field. The final new time level concentration is obtained from this preliminary new time level concentration by an implicit diffusion and reaction half step. The implementation of Smolarkiewicz and Margolin's scheme in the EFDC model is described by Hamrick and Wu (1996).

The next issue to be addressed involves the coupling or linking of the hydrodynamic and water quality models. Hamrick (1994a) reviewed and evaluated techniques for coupling or linking estuarine and coastal hydrodynamic and biogeochemical models. In linking or coupling hydrodynamic and water quality or biogeochemical transport and transformation models, two separate but related issues arise. The first issue involves the spatial and temporal scale relations between the hydrodynamic and water quality models. Four possible spatial and temporal resolution scale relations will be considered: identical spatial and temporal resolution; identical

Assigning a computational score of 10 for the 20 water quality state variable coupled model, the hydrodynamic component alone would have a computational score of (10/3.5) or 2.85 and the water quality component alone would have a computational score of 7.15. If the reduced water quality model were utilized, the water quality component would have a score of 3.2 and the coupled score would be 6.05.

The one to one linking alternative provides the same scores for single runs of embedded and externally linked models. However, during the calibration and verification of a water quality model, numerous water quality simulations might be conducted using the same saved hydrodynamic scenario. If a saved hydrodynamic scenario is used for five water quality simulations, the effective score of the full and reduced water quality models would be (7.15+(2.85/5)) or 7.72 and (3.2+(2.85/5)) or 3.77, respectively. The relevant computational scores are summarized as follows:

Full Water Quality and Simultaneous Hydrodynamics	10.0
Full Water Quality and Saved Hydrodynamics	7.72
Reduced WQ and Simultaneous Hydrodynamics	6.05
Reduced WQ and Saved Hydrodynamics	3.77

These results indicate a reduction in computational requirements if saved hydrodynamics are used for multiple water quality simulations. The EFDC model allows this mode of operation by executing in a transport and transformation mode using saved hydrodynamics. It is noted that the saved hydrodynamics approach becomes less efficient as the sophistication of the water quality model increases. However, the saved hydrodynamics approach is not without drawbacks. First, the saved hydrodynamic transport files may be very large, particularly if seasonal or annual scale simulations are goal. For example, one year of hydrodynamic transport data saved at one hour intervals for a grid having 1000 active horizontal cells and four layers in the vertical would require on the order of 1 gigabyte of storage. Although the cost of this storage is not significant, the water quality with saved hydrodynamics scores should be increased to account for disk access times which can be significant on personal computers. The second drawback is the development of interfacing software if not previously existing, between the independent hydrodynamic and water quality models. Based on the writer's experience, the cost of developing such software would be better spent on computing hardware to handle the higher computational requiresments of simultaneous hydrodynamic and water quality simulation.

The second alternative for linking involves identical spatial resolution (*i.e.*, the same grid) and coarser resolution or a greater time step for the water quality model. This approach has met with some success in estuarine water quality modeling, using tidal cycle and daily averages, where the average velocity over the averaging period is typically an order of magnitude lower than maximum instantaneous velocities, allowing a corresponding order of magnitude increase in the water quality model time step (Dortch *et al.*, 1990; Hamrick, 1994a). The appropriate tidally-averaged velocity has shown to be the Lagrangian mean rather than the traditional Eulerian mean (Hamrick, 1994a). Unfortunately, the Lagrangian mean can only be determined for flow environments that are classified as weakly nonlinear. Although this approach was used for linking CH3D-WES and CE-QUAL-ICM in the first phase of the Chesapeake Bay Modeling program, it has been abandoned in favor of alternative one in the now ongoing second phase. The primary reason for this change is the increased spatial resolution in the second phase. Increased spatial resolution results in more realistic representation of bathymetry and shoreline features and a corresponding increase in nonlinearity of the predicted flow field. The stronger nonlinearity in turn results in the larger residual velocities and a breakdown in the assumptions necessary for calculating the Lagrangian mean velocity field. Given the significance of tide induced residual circulation in the Peconic Bays System (Gomez-Reyes, 1989) and the potential for not being able to determine Lagrangian mean velocities, this alternative is not recommended.

The third alternative for linking or coupling involves identical temporal resolution and coarser spatial resolution in the water quality model. The spatial coarsening generally involves collapsing four or nine horizontal hydrodynamic cells to a single water quality cell or collapsing multiple hydrodynamic layers in the vertical to a single water quality layer. Considering a two-dimensional depth averaged simulation, the four to one collapse would result in one quarter the number of water quality cells and a doubling of the time step. Although this approach is certainly attractive, its primary limitation is loss of realism in the physical transport field which

5. Feasibility of Three-Dimensional Hydrodynamic and Water Quality Modeling of the Peconic Bays System

To estimate the feasibility of a fully coupled hydrodynamic and water quality simulation of the Peconic Bays system on seasonal to annual time scales, the EFDC modeling system was applied to a preliminary grid of the system. The horizontal grid, Figure 4, is composed of approximately 900 square cells, 1 km by 1 km. Six sigma stretched layers were used in the vertical. A time step of 4 minutes was used for the temporal integration. Because the reduced 9 state variable water quality model was not operable at the time of the benchmark runs, the full 20 state variable model was used. The coupled model was run of a 66 MHz Power Macintosh and a 90 MHz Pentium PC compatible. The Macintosh executable was compiled with the Absoft FORTRAN compiler while the PC executable was compiled with the Lahey FORTRAN compiler. The CPU times for one day of execution were 22 and 24 minutes on the Macintosh and PC respectively. Extensive profiling of the EFDC code (Hamrick and Wu, 1966) indicates that on single nonvector processors, the water quality simulation portion of the EFDC mode utilizes approximately 70 per cent of the total CPU time. Scaling the 20 state variable times to 9 state variables gives 13.5 and 14.8 minutes for the Mac and PC, respectively. The lack of significant density stratification in the system suggest that 4 rather than 6 layers would be appropriate for representing vertical variations, and the CPU times can be further reduced by approximately 70 per cent to give 9.5 and 10.4 minutes for the Mac and PC, respectively. The 20 state varibale model executing with 4 layer would require15.4 and 16.8 minutes on the Mac and PC respectively

The target platform for use in the water quality modeling study is a 200 MHz Pentium Pro PC compatible. Although such a system was not available at the time of this study, these systems are now in production. Preliminary performance estimates indicate that the 200 MHz Pentium Pro should be at least 4 times faster than the 90 MHz pentium for floating point intensive computations. Thus a reasonable estimate of 2.6 and 4.2 CPU minutes per day of simulation on the 200 MHz Pentium Pro system is arrived at of the 9 and 20 state variable water quality models, respectively. These estimates translate to approximately 16 and 25 CPU hours per year of simulation for the 9 and 20 state variable models. The execution time for WASP5 water quality model running on the 4 layer, 900 horizontal cell grid, used

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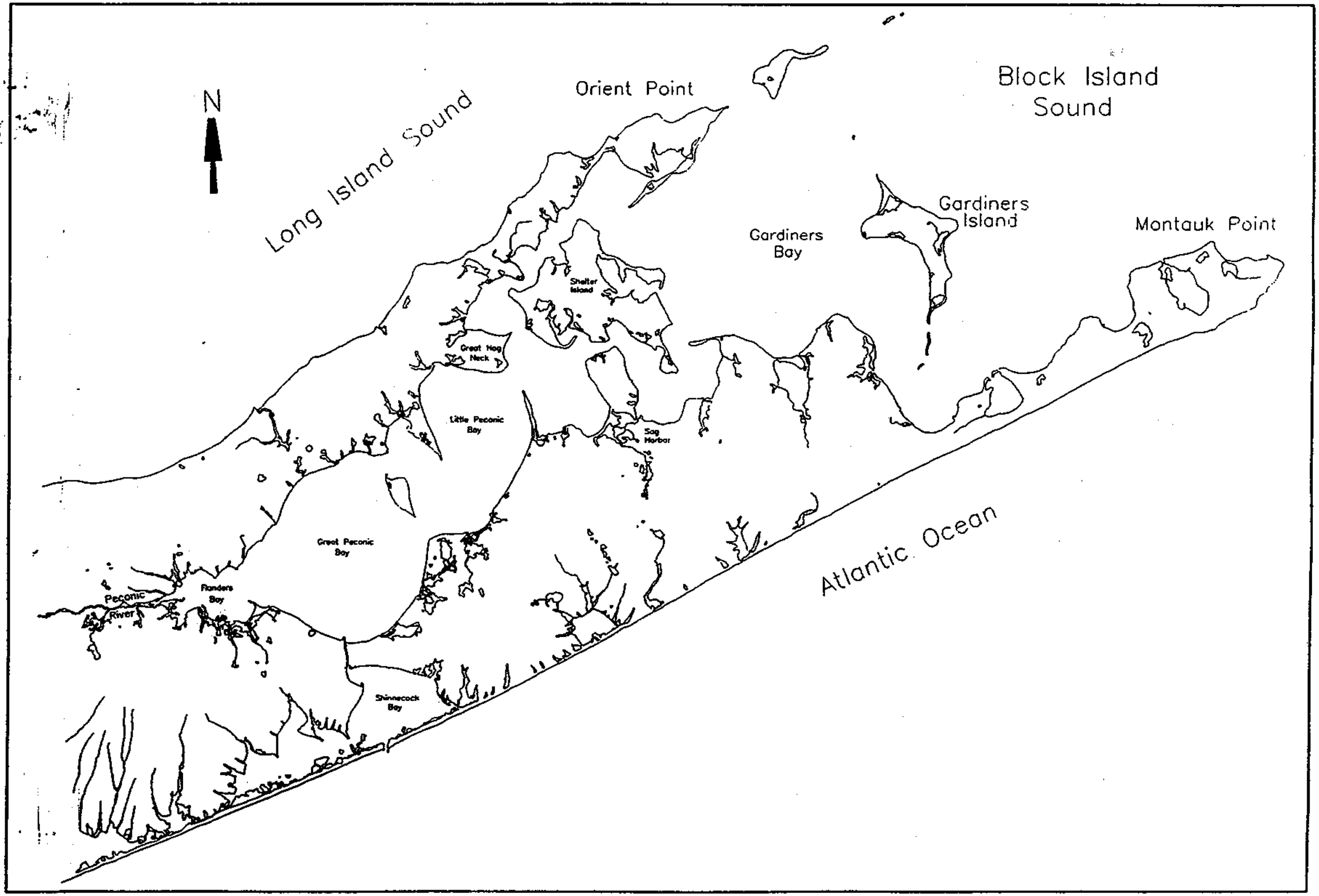
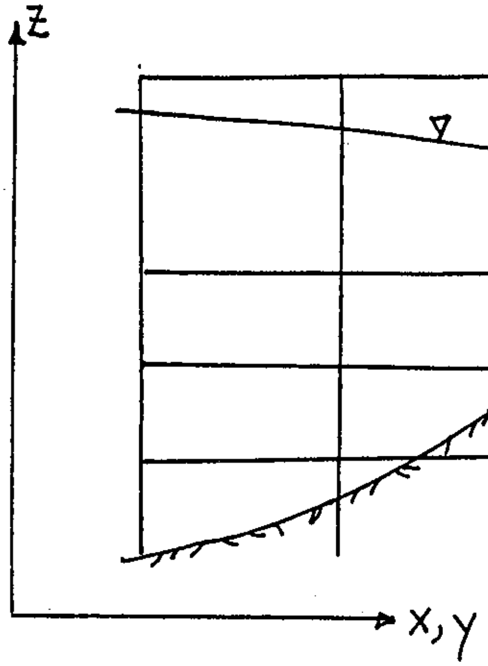
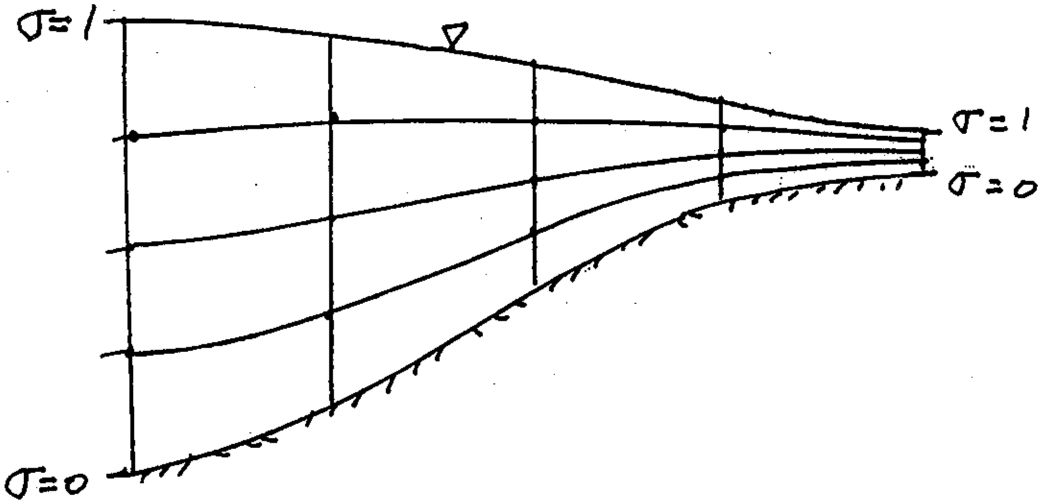


Figure 1. The Eastern Long Island Bays System.



Physical vertical grid



Stretched, sigma or topography following vertical grid

Figure 3. Physical (Cartesian) and stretch or topography following vertical coordinates.

Appendix A

Three-Dimensional Hydrodynamic and Transport Equations

The model equations used in the EFDC model are the horizontal momentum equations:

$$\begin{aligned}&\partial_t(m_x m_y Hu)+\partial_x(m_y Huu)+\partial_y(m_x Hvu)+\partial_z(m_x m_y wu)-f_e m_x m_y Hv\\&=-m_y H\partial_x(p+p_{atm}+\phi)+m_y(\partial_x z_b^{*}+z\partial_x H)\partial_z p+\partial_z\left(m_x m_y \frac{A_v}{H}\partial_z u\right)+Q_x\end{aligned} \tag{A1}$$

$$\begin{aligned}&\partial_t(m_x m_y Hv)+\partial_x(m_y Huv)+\partial_y(m_x Hvv)+\partial_z(m_x m_y wv)+f_e m_x m_y Hu\\&=-m_x H\partial_y(p+p_{atm}+\phi)+m_x(\partial_y z_b^{*}+z\partial_y H)\partial_z p+\partial_z\left(m_x m_y \frac{A_v}{H}\partial_z v\right)+Q_y\end{aligned} \tag{A2}$$

$$m_x m_y f_e = m_x m_y f - u\partial_y m_x + v\partial_x m_y \tag{A3}$$

$$(\tau_{xz},\tau_{yz}) = A_v H^{-1}\partial_z(u,v) \tag{A4}$$

where u and v are the horizontal velocity components in the curvilinear horizontal coordinates x and y, respectively. The scale factors of the horizontal coordinates are mx and my. The vertical velocity in the stretched vertical cooridnate z, is w. The physical vertical coordinates of the free surface and bottom bed are zs^* and zb^* respectively. The total water column depth is H, and ϕ is the free surface potential which is equal to gzs^*. The effective Coriolis acceleration fe incorporates the curvature acceleration terms according to (A3). The Q terms in (A1&A2) represent optional horizontal momentum diffusion terms. The vertical turbulent viscosity Av relates the shear stresses to the vertical shear of the horizontal velocity components by (A4). The kinematic atmospheric pressure, referenced to water density is patm, while the excess hydrostatic pressure in the water column is given by:

$$\partial_z p = -gHb = -gH(\rho-\rho_o)\rho_o^{-1} \tag{A5}$$

where ρ and ρo are the actual and reference water densities and **b** is buoyancy. The three-dimensional continuity equation in the

Appendix B

Tidal Inlet Submodel

The derivation of the tidal inlet submodel starts with either the x or y horizontal momentum equations (A1, A2) with the x equation used here for illustration. The x momentum equation, with the lateral velocity v, set to zero, the surface atmospheric pressure negelected, and the Coriolis and curvature terms omitted due to the assumption of a straight and narrow inlet, is:

$$\begin{aligned}&\partial_t\left(m_yHu\right)+\frac{1}{m_x}\partial_x\left(m_yHuu\right)+\partial_z\left(m_ywu\right)\\&=-\frac{m_yH}{m_x}\partial_x(p+\phi)+\frac{m_y}{m_x}\left(\partial_xz_b^*+z\partial_xH\right)\partial_zp+\partial_z\left(m_y\frac{A_v}{H}\partial_zu\right)\end{aligned}\tag{B1}$$

Inserting the hydrostatic relationship (A5) into the second term on the right side of (B1) gives:

$$\begin{aligned}&\partial_t\left(m_yHu\right)+\frac{1}{m_x}\partial_x\left(m_yHuu\right)+\partial_z\left(m_ywu\right)\\&=-\frac{m_yH}{m_x}\partial_x(p+\phi)-\frac{m_y}{m_x}\left(\partial_xz_b^*+z\partial_xH\right)gHb+\partial_z\left(m_y\frac{A_v}{H}\partial_zu\right)\end{aligned}\tag{B2}$$

The hydrostatic relationship (A5) is integrated from an arbitrary z level to the free surface, $z=1$, to give:

$$p=gH\int_z^1 bdz\tag{B3}$$

Inserting (B3) into (B2) gives:

$$\begin{aligned}&\partial_t\left(m_yHu\right)+\frac{1}{m_x}\partial_x\left(m_yHuu\right)+\partial_z\left(m_ywu\right)\\&=-\frac{m_yH}{m_x}\partial_x\phi-g\frac{m_yH}{m_x}\partial_x\left(H\int_z^1 bdz\right)-g\frac{m_yH}{m_x}\left(\partial_xz_b^*+z\partial_xH\right)b+\partial_z\left(m_y\frac{A_v}{H}\partial_zu\right)\end{aligned}\tag{B4}$$

Neglecting volume storage in the inlets gives:

$$\begin{aligned}&\partial_t Q+\frac{1}{m_x}(uQ)_d-\frac{1}{m_x}(uQ)_u\\&=-\frac{m_y H}{m_x}(1+b)(\phi_d-\phi_u)-g\frac{m_y}{m_x}\frac{H^2}{2}(b_d-b_u)-m_y\overline{\tau}_b\end{aligned} \tag{B10}$$

The surface elevation potential in the grid cell upstream of the inlet entrance is related to the entrance value ϕu by:

$$\phi_U=\phi_u+\alpha_u\frac{u_u^2}{2} \tag{B11}$$

where αu is the entrance loss coefficient. The elevation potential downstream grid cell is related to the downstream inlet exit potential ϕd by:

$$\phi_d=\phi_D+\alpha_d\frac{u_d^2}{2} \tag{B12}$$

where αd is the exit loss coefficient. Substituting (B11&B12) into (B10) gives:

$$\begin{aligned}&\partial_t Q+\frac{1}{m_x}(uQ)_d-\frac{1}{m_x}(uQ)_u=-\frac{m_y H}{m_x}(1+b)(\phi_D-\phi_U)\\&-\frac{m_y H}{m_x}(1+b)\left(\alpha_d\frac{u_d^2}{2}+\alpha_u\frac{u_u^2}{2}\right)-g\frac{m_y}{m_x}\frac{H^2}{2}(b_d-b_u)-m_y\overline{\tau}_b\end{aligned} \tag{B13}$$

Assuming the upstream and downstream velocities uu and ud, are equal, that $myHu$ is equal to Q, and introducing a quadratic bottom stress law gives:

$$\begin{aligned}&\partial_t Q=-\frac{m_y H}{m_x}(1+b)(\phi_D-\phi_U)-\frac{1}{m_x}\left(\alpha_d\frac{u_d Q}{2}+\alpha_u\frac{u_u Q}{2}\right)\\&-g\frac{m_y}{m_x}\frac{H^2}{2}(b_d-b_u)-m_y c_b|\overline{u}|\overline{u}\end{aligned} \tag{B14}$$

where cd is the dimensionless bottom stress coefficient.