A BAY/ESTUARY MODEL TO SIMULATE HYDRODYNAMICS AND WATER QUALITY TRANSPORT: PART 1: HYDRODYNAMICS

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ABSTRACT

This paper presents the development and application of a bay/estuary model to simulate hydrodynamics and thermal and salinity transport. The hydrodynamic module solves three-dimensional Navier-Stokes equations with or without the hydrostatic assumptions. The turbulence is modeled with the generic length scale (GLS) turbulence transport equations. The Boussinesq approximation is employed to deal with the buoyancy force due to temperature and salinity variations. The moving free surface is explicitly handled by solving the kinematic boundary condition equation using a node-repositioning algorithm. The transport module solves the energy equation for spatial-temporal distributions of temperature and the mass transport equations for the salinity field. The Arbitrary Lagrangian-Eulerian (ALE) representation is adopted for all transport equations including momentum transport. The solution is obtained with finite element methods or a combination of finite element and Semi-Lagrangian (particle tracking) methods. The model has been successfully calibrated with tides and salinities and is applied to Loxahatchee Estuary for the investigation of its minimum flow requirements to maintain ecological balance.

1. INTRODUCTION

Over the past few years, there has been growing demanding of three-dimensional hydrodynamics models in estuarine studies. However, the majority of these models are based on the multi-layer or the multi-level approaches (Drago et al., 2000; Kim et al., 1994; Shankar et al., 1997; and Zhang et al., 2000). In the multi-layer approach, the column of water is divided into layers that can move freely in the vertical direction to maintain continuity, but there is no transport across layers. Furthermore, the application of multi-layer model to simulate tidal currents requires the strict specification of open boundary conditions at the layer interfaces, which is rather difficult to obtain in practical situations. The multi-level model, on the other hand, describes the vertical motion of fluid in terms of vertical transport between the various levels, while the interfaces between the layers are fixed in space. Compared to fully three-dimensional models, multi-level modeling is not convenient in areas where high vertical gradient of density are present. As a matter of fact, both multi-layer model and multi-level model are composed of a stacking of many depth-averaged hydrodynamic models in the vertical direction. Within each layer, the hydrostatic assumption and the depth-integration are still required. Sometimes a fully three-dimensional hydrodynamic model based on the Navier-Stokes equations is needed in order to provide reliable description of convective dynamics. As it is commonly believed that the Navier-Stokes equations are the general governing equations for fluid flows, a model rooted in the Navier-Stokes equations is valid for flow motions over a large range of length-scales.

In this paper we present a bay/estuary surface water model to simulate hydrodynamics and thermal and salinity transport. The hydrodynamic module is based on the three-dimensional Navier-Stokes equations with or without the hydrostatic assumptions. The transport module solves the energy equation for spatial-temporal distributions of temperature and the mass transport equations for the salinity field. The Arbitrary Lagrangian-Eulerian (ALE) representation (Chan, 1975) is adopted for all transport equations. A moving grid method based on node-repositioning is used to track the change of water level. The model has been successfully calibrated with tides and salinities and is applied to Loxahatchee River and Estuary for the investigation of its minimum flow requirements to maintain ecological balance.

This paper is arranged as follows. In Section 2, we state the underlying mathematical model, including the governing equations and the numerical methods. Section 3 presents the application of the model to Loxahatchee River and Estuary and compares the model output with the field data. Conclusion is given in Section 4.

2. MATHEMATICAL MODEL

The governing equations, boundary conditions, and numerical methods of the surface water model are briefly introduced in this section.

2.1 Governing equations.

In modeling the flow problem with free surface, the moving grid method is used in combination with the Arbitrary Lagrangian-Eulerian (ALE) representation (Chan, 1975) of the governing equations. The moving grid approach allows the mesh to move to accommodate the deformation of the free surface and the movement of the mesh node does not necessarily follow the motion of fluid particle. Namely the mesh can move arbitrarily to fit the free surface. The ALE representation can be converted to Lagrangian or Eulerian representations (Braess & Wriggers, 2000). The ALE representation adopts a notation "$d\Phi/dt$" for the total derivative of Φ. The Eulerian derivative denoted by "$\partial\Phi/\partial t$" is related to the total derivative in the form of $\frac{d\Phi}{dt} = \frac{\partial\Phi}{\partial t} + (\vec{V}_g \cdot \nabla)\,\Phi$ with $\vec{V}_g$ representing the grid moving velocity.

The three-dimensional Navier-Stokes equations include the continuity equation

$$\nabla \cdot \vec{V} = Q, \tag{1}$$

and the momentum equation in the ALE form

$$\begin{aligned} &\frac{d\vec{V}}{dt} + (\vec{V} - \vec{V}_g) \cdot \nabla\vec{V} + (\nabla \cdot \vec{V})\vec{V} = \\ &-\nabla\left(\frac{p}{\rho_0} + g\,z\right) - \frac{\Delta\rho}{\rho_0} g\nabla z + \frac{1}{\rho_0}\nabla \cdot \vec{\vec{\tau}} - 2\vec{\Omega} \times \vec{V} + Q\vec{V}_* \end{aligned} \tag{2}$$

where $\vec{V}$ is the flow velocity, Q is the source/sink term, p is the pressure, ρ_0 is the reference density of water, g is the gravitational acceleration. $2\vec{\Omega}\times\vec{V}$ is the Coriollis force, $\vec{V}_*$ is the velocity of source flow, and $\bar{\bar{\tau}}$ is the turbulence stress tensor. The Boussinesq approximation is employed to deal with the buoyancy force reflected by $\Delta\rho$ which is the change of density due to temperature and salinity.

The transport equation for temperature in the ALE form is given by

$$\frac{dT}{dt} + (\vec{V}-\vec{V}_g)\cdot\nabla T + (\nabla\cdot\vec{V})T = \nabla\cdot(K_t\nabla T) + QT_* , \quad (3)$$

where T is the water temperature, T_* is the water temperature of source, and K_t is the thermal diffusivity. Similarly, the transport equation for salinity can be written in the ALE form as

$$\frac{dS}{dt} + (\vec{V}-\vec{V}_g)\cdot\nabla S + (\nabla\cdot\vec{V})S = \nabla\cdot(K_s\nabla S) + QS_* , \quad (4)$$

where S is the salinity, K_s is the saline diffusivity, and S_* is salinity of source.

The similarities between many two-equation closures turbulence models lead to a generalized formulation – the generic length scale (GLS) turbulence model (Umlauf et al., 2003; and Warner et al., 2005), which includes two equations. The first equation is the standard transport equation for turbulent kinetic energy

$$\frac{\partial k}{\partial t} + (\vec{V}-\vec{V}_g)\cdot\nabla k = \frac{\partial}{\partial z}\left(\frac{K_M}{\sigma_k}\frac{\partial k}{\partial z}\right) + P_t + B_t - \varepsilon , \quad (5)$$

where k is the turbulent kinetic energy, ε is the dissipation rate of turbulent kinetic energy, σ_k is the turbulence Schmidt number for k. P_t and B_t represent turbulent production due to shear and buoyancy, respectively. $K_M = c\sqrt{2k}\, l\, S_M + \nu$, where S_M is the stability function describing the effects of shear, ν is the molecular viscosity, c is a constant coefficient, and l is the turbulent length scale, The second equation of the GLS model is the transport equation for a generic parameter ψ

$$\frac{\partial \psi}{\partial t} + (\vec{V}-\vec{V}_g)\cdot\nabla \psi = \frac{\partial}{\partial z}\left(\frac{K_M}{\sigma_\psi}\frac{\partial \psi}{\partial z}\right) + \frac{\psi}{k}(c_1 P_t + c_3 B_t - c_2\,\varepsilon\, F_{wall}) , \quad (6)$$

where σ_ψ is turbulence Schmidt number for ψ, F_{wall} is the wall function, c_1, c_2, and c_3 are constants. Interested reader should refer to Umlauf et al.(2003) and Warner et al.(2005) for more details.

The time evolution of the free water surface elevation is governed by the following equation representing a kinematic boundary condition, which states the fact that the free surface is a material surface, i.e., the fluid particles initially locate on the free surface always remain on the surface. The free surface elevation equation is given by

$$\frac{d\eta}{dt} + (u_s - u_g)\frac{\partial\eta}{\partial x} + (v_s - v_g)\frac{\partial\eta}{\partial y} = w_s + R - E , \quad (7)$$

where η is the free surface elevation with respect to a reference elevation H_0 as defined in Figure 1. $u_s, v_s,$ and w_s are the three components of velocity on the free surface. u_g and v_g are the horizontal components of the moving grid velocity on the free surface. R and E represent the rainfall and evaporation intensity, respectively.

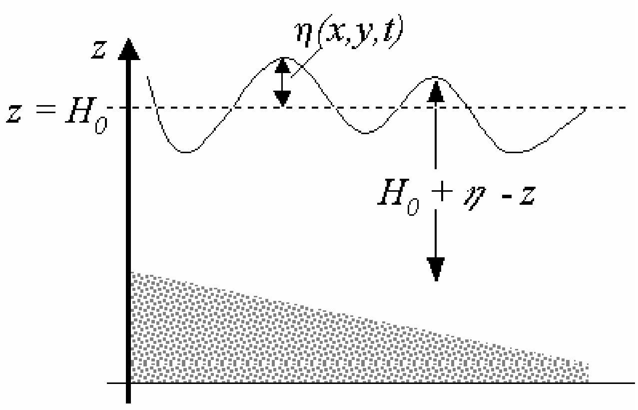


FIGURE 1. Schematic Sketch of Free Surface

Equations (1), (2), and (7) can be used to derive the continuity equation and momentum equations of the hydrostatic model.

2.2 Boundary conditions.

A complete system should include Equations (1)-(7) above and some of the following boundary conditions.

The The general form of the Dirichlet boundary condition is given by $\vec{\Psi}\Big|_{\Gamma_D} = \vec{q}_D$ where $\vec{\Psi} = \{p, u, v, w, \eta, T, S, k, \psi\}^T$ is the solution vector. Γ_D indicates the boundary where the Dirichlet boundary condition is specified.

The conservation of momentum at free surface leads to the dynamic boundary condition, under the assumption that the surface tension is negligible and the pressures on both sides of the air-water interface are equal, $\vec{n}\cdot\bar{\bar{\tau}} = \vec{n}\cdot\bar{\bar{\tau}}_{wind}$ where $\vec{n}$ is the outward-pointing unit normal vector on the free surface, and $\bar{\bar{\tau}}_{wind}$ is the wind stress at water surface. A similar boundary condition can be used for river bottom $\vec{n}\cdot\bar{\bar{\tau}} = \vec{n}\cdot\bar{\bar{\tau}}_{bed}$ where $\vec{n}$ is the outward-pointing normal unit vector on the river bed, and $\bar{\bar{\tau}}_{bed}$ is the river bed stress.

In modeling free surface water body with moving grid method, a moving contact surface is defined as the interface between the water and the sidewall of river bank. The mesh nodes located on the interface should be free to move along the tangent to the interface. Therefore, the standard no-slip boundary condition cannot be used on moving contact surface. We utilize the perfect slip condition $\vec{n}\cdot\vec{V}\Big|_{\Gamma_M} = 0$ where Γ_M indicates the moving contact boundary. $\vec{n}$ is the unit normal vector of the contact surface.

Other boundary conditions may include the flux boundary conditions for temperature, salinity, turbulent kinetic energy and dissipation, and the radiation boundary condition for water elevation.

2.3 Numerical methods and code validation.

The system of the above governing equations and boundary conditions are solved numerically by finite element method or a combination of finite element and Semi-Lagrangian (particle tracking) methods. The commonly adopted standard Galerkin finite element method (GFEM) exhibits global spurious oscillations when the flow is dominated by convection. To avoid the numerical oscillation, a Petrov-Galerkin finite element method (PGFEM) known as the Streamline Upwind Petrov-Galerkin (SUPG) method (Brooks, et al., 1982) is utilized. A fractional-θ-scheme method is used for time discretization with $\theta = 0.5$. In the Semi-Lagrangian method, a particle tracking technique based on element refinement is used to identify the trajectories of fluid particles (Cheng et al., 1996).

The model has been verified through several classical testing cases, including the lid driven cavity flow, the natural convection of cavity flow, the linear sloshing problem, and three-dimensional nonlinear sloshing problem (Shan & Yeh, 2004).

3. LOXAHATCHEE RIVER MODEL

3.1 Study area and model setup.

The study area is the watershed of the Loxahatchee River located on the east coast of Florida within northern Palm Beach and southern Martin Counties. The model domain includes all the major tributaries of the river: the North Fork, Southwest Fork, the Northwest Fork, and the North and South Intracoastal Waterways. An aerial picture of the study area is shown in Figure 2, where the model mesh is plotted on top of the picture. A part of the Atlantic Ocean to the east of Florida coastal line is also included in the model domain to incorporate the tidal boundary condition more precisely. The mesh shown in Figure 2 is used as the base to generate the three-dimensional model mesh which consists of four layers of elements extended from the river bed to the river surface with grid nodes uniformly distributed in the vertical direction. The three-dimensional mesh includes 4936 elements and 30664 quadratic nodes. The horizontal element size ranges from 3500 ft in the Atlantic Ocean to about 15 ft near the Kitching Creek. The South Florida Water Management District (SFWMD) has collected water elevation and salinity data with a frequency of 15 minutes at the following stations in the model domain: Coastal Guard Dock (CGD), Pompano Drive (PD), and Boy Scout Dock (BSD), as marked in Figure 2.

Tide is the major driving force of the surface water system in model domain. Because no tidal data is available at the ocean boundary of the model, we extrapolated the water elevation data at CGD to the ocean boundary with a time shift and amplitude adjustment. The fresh water inflow at the upstream of the tributaries of the river is determined from field data. A constant salinity of 35.5 ppt is set at the ocean boundary. Precipitation and evaporation are not considered in the current model run. The coupling between the surface and groundwater is not included in the model as presented. An integrated surface and subsurface model has been developed and will be presented elsewhere.

3.2 Model output.

The model calibration was initiated from a cold start (time $t = 0$) with uniform water stage and zero salinity in the model domain. It took 12-16 tidal cycles for the flow and distribution of salinity to reach a fully developed stage. Figure 3 shows the distribution of salinity in the model domain when $t = 333$ hours.

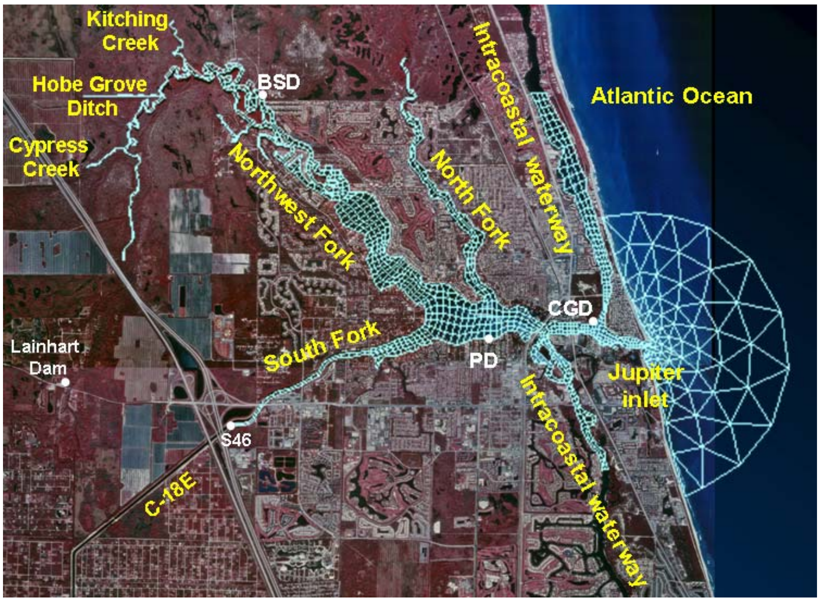


FIGURE 2. Aerial picture of the Loxahatchee River and Estuary and model mesh.

During the model run, the time history of water stage and salinity at stations of CGD, PD, and BSD were recorded and compared with the field data. The results are displayed in Figures **Error! Reference source not found.**, **Error! Reference source not found.**, and 6. In all these figures, solid line represents the mode output (M), and the corresponding field data (F) is plotted in dashed line. Figure **Error! Reference source not found.**(a) compares the model output water stage and with the field data at CGD. The comparison of salinity at the same station is shown in Figure **Error! Reference source not found.**(b). The model output and field data at stations PD and BSD are displayed in Figures **Error! Reference source not found.** and 6, respectively. Overall, very good agreement is found between the model output and field data for water stage. The model output salinity also agrees reasonably well with the field data at all three stations. The quantitative error measurement of model prediction is given in Table 1, where *rms* stands for the root-mean-squared error and R^2 is the Pearson product-moment correlation coefficient.

TABLE 1. Prediction error measurement

Location	**Water Stage**		**Salinity**	
	rms	R^2	***Rms***	R^2
Coastal Guard Dock (CGD)	5.20×10^{-2}	0.9963	1.19×10^{0}	0.6780
Pompano Drive (PD)	2.52×10^{-1}	0.8904	2.07×10^{0}	0.4210
Boy Scout Dock (BSD)	2.43×10^{-1}	0.8983	3.88×10^{0}	0.6851

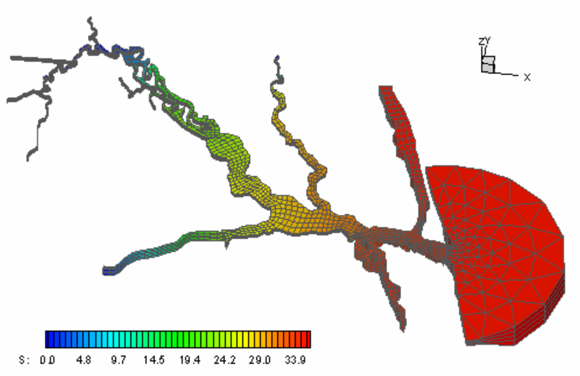
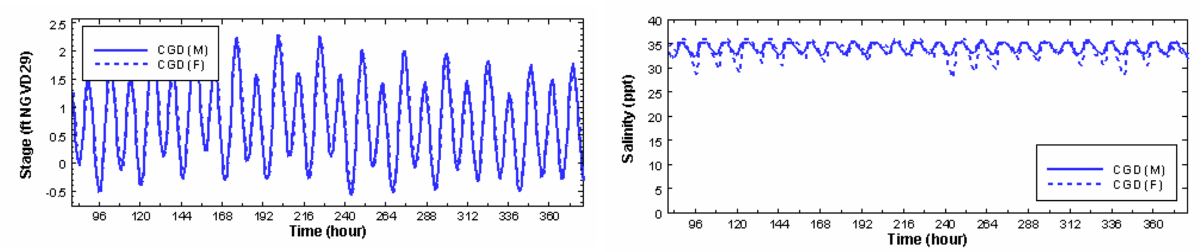
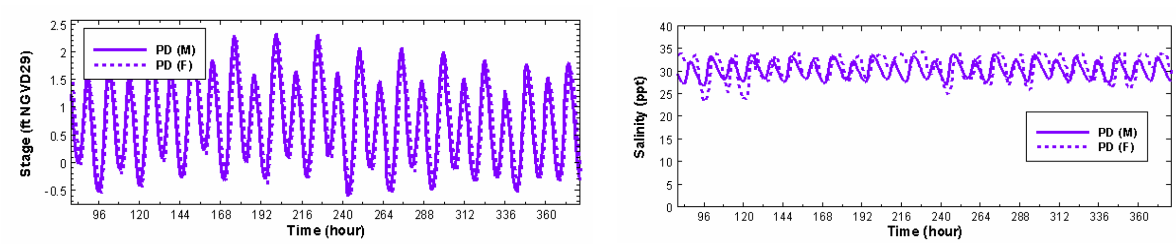


FIGURE 3. Distribution of salinity at t = 333 hour.



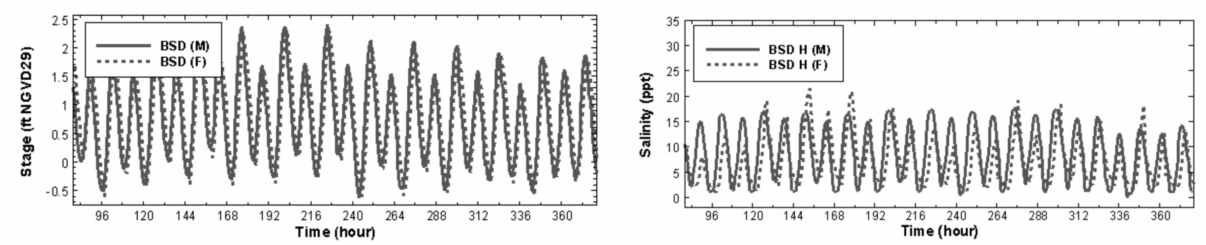
(a) water stage (b) salinity

FIGURE 4. Model output at CGD in comparison with field data.



(a) water stage (b) salinity

FIGURE 5. Model output at PD in comparison with field data.



(a) water stage (b) salinity

FIGURE 6. Model output at BSD in comparison with field data.

4. CONCLUSION

We have developed a three-dimensional hydrodynamics and transport model for bay/estuary based on Navier-Stokes equations in ALE form combined with the moving grid approach. The numerical solution is obtained using finite element method in a possible combination with the Semi-Lagrangian (particle tracking) method. The model has been successfully calibrated against field tidal and salinity data and is applied to Loxahatchee Estuary for the investigation of its minimum flow requirements to maintain ecological balance. The future work may include the development an integrated surface/subsurface model for the study area.

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