AN INTEGRATED THREE-DIMENSIONAL SURFACE WATER AND GROUNDWATER MODEL TO SIMULATE HYDRODYNAMICS AND THERMAL AND SALINITY TRANSPORT

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ABSTRACT: This paper presents the development and application of an integrated surface water and groundwater model to simulate hydrodynamics and temperature and salinity in tidal water bodies and subsurface media. The hydrodynamic module for tidal waters solves three-dimensional Navier-Stokes equations with or without the hydrostatic assumptions. The Richards equation is used to simulate the subsurface flow in variably varied saturated media. 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 temperature distribution and a mass transport equation for salinity fields. 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 is developed for application to Loxahatchee Estuaries to investigate the minimum flow requirements to maintain ecological balances.

1. INTRODUCTION

Numerical simulations have proved a very useful tool for coast engineering, environmental protection, and disaster planning. The accurate predication relies on appropriately modeling of tides, currents, and salinity and temperature distribution as well as dispersion of pollutants. The past decades have seen the rapid development of three-dimensional hydrodynamic computer codes (e.g., EFDC by Harick, 1992; CH3D by Sheng, 1990; UnTRIM by Casulli and Zanolli, 1998; 3D ADCIRC by Leuttich and Weterink, 2001; RMA10 by King, 1988; and ECOM by Blumberg and Mellor, 1987) for the investigation of flow field in coastal areas. However, most of these codes invoke the hydrostatic assumptions which could have enormous errors in both phases and amplitudes of tides and currents for many situations (Wu, 2003). In order to provide reliable description of convective dynamics in the coastal region, a fully three-dimensional hydrodynamic model based on the Navier-Stokes equations is needed. 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. Traditionally it is a widely held belief that the models based on three-dimensional Navier-Stokes equations are too expensive to use for the computation of the coastal flow. However, due to the remarkable progress in computing facilities as well as techniques of computational fluid dynamics (CFD), the modeling of coastal flow based on three-dimensional Navier-Stokes equations becomes a feasible task.

Field measurements in the Loxahatchee river study area indicate that the links between groundwater and the estuary are very dynamic. Therefore, it becomes obvious that a model fully integrating both surface water and groundwater components is necessary. Such a model can be used to simulate the dynamic exchanges between the estuarine river and the surfacial aquifer in a fully coupled manner.

This paper is organized as follows. Section 2 gives a brief review of the governing equations and boundary conditions for surface water bodies. Governing equations and associated boundary conditions for subsurface flow are introduced in Section 3. Numerical solution options are outlined in Section 4. Section 5 presents a rigorous couple strategy between surface water and subsurface flows. A preliminary test run of the model application to the Loxahatchee River of Florida is given in Section 6.

2. SURFACE WATER MODEL

Governing Equations: The governing equations of the hydrodynamics are the three-dimensional Navier-Stokes equations for incompressible flow. The equation for the conservation of fluid mass, or the continuity equation is

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

where $\vec{V}$ is the flow velocity, Q is the source/sink. The equation of conservation of momentum is the modified Navier-Stokes equation

$$\frac{\partial \vec{V}}{\partial t} + \vec{V}\cdot\nabla\vec{V} + (\nabla\cdot\vec{V})\vec{V} = -\nabla(\frac{p}{\rho_o} + g\,z) - \frac{\Delta\rho}{\rho_o} g\,\nabla z + \frac{1}{\rho_o}\nabla\cdot\bar{\bar{\tau}} - 2\vec{\Omega}\times\vec{V} + Q\vec{V}_* \tag{2}$$

where p is the pressure, ρ_o 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 flow associated with the source, and $\Delta\rho = \rho_o\,(1-\alpha\,\Delta T + \beta\,\Delta S)$ is the change of density due to temperature and salinity variation (where $\Delta T = T - T_o$ and $\Delta S = S - S_o$; T_o and S_o are the reference temperature and salinity, respectively; α is the thermal expansion coefficient; β is the saline expansion coefficient). The viscous stress tensor $\bar{\bar{\tau}}$ in Eq. **Error! Reference source not found.** is related to the strain tensor by $\bar{\bar{\tau}} = 2\rho_o\,\nu\bar{\bar{\varepsilon}}$ (where $\bar{\bar{\varepsilon}} = [\,\nabla\vec{V} + (\nabla\vec{V})^T\,]/2$ is the strain rate tensor and ν is the kinetic viscosity).

The time evolution of the free surface elevation is governed by a kinematic equation as follows:

$$\frac{\partial\eta}{\partial t} + u_s\frac{\partial\eta}{\partial x} + v_s\frac{\partial\eta}{\partial y} = w_s + R - E \tag{3}$$

where η is the tide; u_s, v_s, w_s are the three components of velocity on the free surface; R is the rainfall intensity; and E is the evaporation intensity

The transport equations include a temperature equation and a salinity equation. The temperature equation is derived from the conservation of energy as

$$\frac{\partial T}{\partial t} + \vec{V}\cdot\nabla T + (\nabla\cdot\vec{V})T = \nabla\cdot(\frac{\bar{\bar{\kappa}}}{\rho_o C_w}\bullet\nabla T) + QT_* \tag{4}$$

where T is the water temperature, $\bar{\bar{\kappa}}$ = the thermal conductivity/dispersion tensor, C_w is the specific heat of water, and T is the temperature of the source water.

The salinity equation can be derived based on conservation of mass as

$$\frac{\partial S}{\partial t} + \vec{V}\cdot\nabla S + (\nabla\cdot\vec{V})S = \nabla\cdot(\bar{\bar{K}}_s\bullet\nabla S) + QS_* \tag{5}$$

where S is the salinity, $\bar{\bar{K}}_s$ is the saline diffusivity/dispersion tensor, and S_* is the salinity of the source water.

<u>Boundary Condition</u>: Equations (1), (2), (4), and (5) apply everywhere within the fluid domain subject to boundary conditions. The general form of the Dirichlet boundary condition is given by

$$\bar{\Psi}\Big|_{\Gamma_D} = \bar{\Psi}_D \tag{6}$$

where $\bar{\Psi} = \{p, u, v, w, \eta, T, S\}^T$ is the solution vector and Γ_D indicates the boundary where the Dirichlet boundary condition is specified. Note the Dirichlet boundary may locate differently for different state variables.

On the free surface, the conservation of mass is guaranteed by the kinematic equation of free-surface elevation. The conservation of momentum at free surface leads to the following dynamic boundary condition, if the surface tension is negligible:

$$\vec{n}\cdot\bar{\bar{\sigma}} = \vec{n}\cdot\bar{\bar{\sigma}}_{ext} \tag{7}$$

where $\vec{n}$ is the unit vector normal to free surface and pointing outward the computational domain; $\bar{\bar{\sigma}}$ is stress tensor of the fluid side in the computational domain, e.g. the stressor tensor of water; $\bar{\bar{\sigma}}_{ext}$ is stress tensor of the external fluid, such as air. In Cartesian coordinate system the stress tensor is expressed as

$$\bar{\bar{\sigma}} = [\rho \nu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - p\delta_{ij}] \vec{e}_i \vec{e}_j \tag{8}$$

The moving contact surface is the interface between the fluid and solid wall on which the free surface may slide. To allow the free surface slide along the contact surface, one cannot impose the no-slip boundary condition. In this model, either the perfect slip boundary condition or the Navier's condition is specified on moving contact surfaces:

$$\vec{n} \cdot \vec{V} \Big|_{\Gamma_M} = 0 \quad \text{or} \quad [(\bar{\bar{I}} - \vec{n}\vec{n}) \cdot (\vec{n} \cdot \bar{\bar{\tau}}) + \rho (\bar{\bar{I}} - \vec{n}\vec{n}) \cdot \vec{V}] \Big|_{\Gamma_M} = 0 \tag{9}$$

where Γ_M indicates the moving contact boundary, $\vec{n}$ is the unit normal vector of the contact surface.

The flux boundary for temperature and salinity given by the following equations are imposed at inflow/outflow boundaries.

$$\rho_o C_w \vec{n} \cdot (\vec{V} T - \kappa \nabla T) \Big|_{\Gamma_{IO}} = q_T \quad \text{and} \quad \rho_o \vec{n} \cdot (\vec{V} S - K_s \nabla S) \Big|_{\Gamma_{IO}} = q_S \tag{10}$$

Here Γ_{IO} indicates the inflow/outflow boundary and $\vec{n}$ is the unit normal vector of the boundary.

The thermal energy budget condition at free surface is given as

$$\rho_o C_w \vec{n} \cdot (\vec{V} T - \bar{\bar{\kappa}} \bullet \nabla T) = q_E + q_C + \varepsilon_w \sigma T^4 - (R_{sn} + R_{an}) \tag{11}$$

q_E is the heat flux due to evaporation, q_C is the heat flux due to diffusion, ε_w is the emissivity of water surface ($\varepsilon_w \approx 0.97$), σ is the Stefan-Boltzmann constant (5.67×10^{-8} W m^{-2} K^{-4}), R_{sn} is the net solar radiation, and R_{an} is the net atmospheric radiation.

3. SUBSURFACE MEDIA MODEL

Governing Equations: The governing equations of subsurface flow is the classical Richards' equation modified for the density effect as

$$\frac{\rho}{\rho_o} F \frac{\partial h}{\partial t} = \nabla \cdot \left[\bar{\bar{K}} \cdot \left(\nabla h + \frac{\rho}{\rho_o} \nabla z \right) \right] + \frac{\rho^*}{\rho_o} q \tag{12}$$

where ρ is the fluid density, h is the pressure head with respect to ρ_o, $\bar{\bar{K}}$ is the hydraulic conductivity tensor, q is the flow rate of source/sink, ρ^* is the fluid density of the source/sink, and F is a generalized storage coefficient given by

$$F = \alpha' \frac{\theta}{n_e} + \beta' \theta + n_e \frac{dS}{dh} \tag{13}$$

in which α' is the modified compressibility of the media, θ is the effective moisture content, n_e is the effective porosity, β' is the modified compressibility of water, and S is the degree of saturation. The flow velocity is given by Darcy's law as

$$\vec{V} = -\bar{\bar{K}} \cdot \left(\frac{\rho_o}{\rho} \nabla h + \nabla z \right) \tag{14}$$

The transport equations include a temperature equation and a salinity equation. The temperature equation is derived from the conservation of energy as

$$\frac{\partial\,[(\rho_w C_w \theta + \rho_b C_m)T}{\partial t} + \nabla\bullet(\rho_w C_w \bar{V} T) - \nabla\cdot(\bar{\bar{D}}^H \bullet \nabla T) = H^a + H^r \tag{15}$$

where ρ_w is the water density, C_w is the specific heat of water, ρ_b is the bulk density of the media, C_m is the specific heat of the media, $\bar{\bar{D}}^H$ is the apparent thermal conductivity/dispersion tensor, H^a is the artificial heat source, and H^r is the artifical heat source due to rainfall.

The salinity equation can be derived based on conservation of mass as

$$\frac{\partial\,\theta S}{\partial t} + \nabla\cdot(\bar{V}S) - \nabla\cdot(\theta\bar{\bar{D}}\bullet\nabla S) = S^{as} \tag{16}$$

where $\bar{\bar{D}}$ is the diffusion/dispersion coefficient tensor and S^{as} is the artificial salt source.

<u>Boundary Conditions</u>: Equations (12) through (14) and the constitutive relationships among the pressure head, degree of saturation, and hydraulic conductivity tensor, together with associated and appropriate initial conditions and boundary conditions, can be used to compute the temporal-spatial distributions of the hydrological variables, including pressure head, total head, effective moisture content, and Darcy's velocity. Four basic types of boundary conditions and a river boundary condition can be specified for variably saturated flows. In addition, a variable boundary condition normally encountered at the air-media interface is stated. These varieties of boundary conditions are included here to handle a variety of physical phenomena that can happen on the global boundary. These boundary conditions are described below.

The first type of boundary conditions is the Dirichlet condition where the pressure is prescribed. For instance, the bottom surface of a river or a lake can be defined as a Dirichlet boundary of the hydrologically connected subsurface system and the water depth can be used as the pressure head on the boundary under the hydrostatic assumption. The second type is the Cauchy condition where the volumetric flux is given. For example, the infiltration rate on the ground surface or through the bottom of hydraulically non-connected surface water bodies can be considered as a Cauchy boundary if the infiltration rate is measured. The third type is the Neumann condition where the flux due to pressure gradient is known. On the drainage boundary, for example, the flux is due to gravity and it can be considered as a Neumann boundary with a zero Neumann flux. The fourth type is the global river boundary condition. If there are sediment layers around the wet parameter of the river-media interfaces, then flux depends on both the depth of river, properties of sediment layers, and pressure head beneath the river. Under such circumstances, a radiation type of conditions can be imposed.

The fifth type is the variable condition. On a variable boundary, which is normally the air-media interface, infiltration, ponding, or seepage can occur during precipitation periods. The throughfall can either completely or partially penetrate into the subsurface system, depending on the soil condition. For the complete penetration, a Cauchy-type condition is used, while a Dirichlet-type condition is employed for the partial penetration when either a ponding or a surface runoff occurs. During non-precipitation periods, three situations are possible: a ponding condition may still exist in the early stage, followed by soil evaporation for a period of time, and finally a dry condition can be reached if the period is long enough. These physical conditions lead to the specification of either the Dirichlet type with ponding depth or minimum pressure or the Cauchy type with potential evapotranspiration. At the subsurface-atmosphere interface, the boundary condition for thermal transport must satisfy the energy budget condition similar to that for surface water-atmosphere interface.

4. NUMERICAL METHODS

<u>Finite Element Method</u>: Three types of elements are used for spatial discretization: the hexahedral element, the triangle-based prism element, and the tetrahedral element. Each element is linear or quadratic depending on the primitive variables. Within each element, the primitive variables are approximated by the appropriate interpolation functions. For viscous incompressible flow problems governed by Navier-Stokes equations, the interpolation

function for velocity and pressure must satisfy the Ladyzhenskaya-Babuska-Brezzi (LBB) condition that requires the pressure interpolation function being at least one order lower than that for velocity. Thus, in the surface water model, pressure, temperature, and salinity are approximated with first order element while the velocity is discretized with quadratic elements. In the subsurface model, only linear elements are used.

The standard Galerkin finite element method (GFEM) is commonly adopted to solve fluid mechanics problem. As it is well know, the numerical solution of Navier-Stokes equation using GFEM formulation exhibits global spurious oscillations when the flow is dominated by convection. To avoid the numerical oscillation, the Petrov-Galerkin finite element (PGFEM) should be used. In PGFEM, the weighting function is the same for all terms, except for the convection term. For the convection terms, the weighting function is normally one or two order higher than the interpolation function. In this study, a PGFEM known as the streamline upwind Petrov-Galerkin (SUPG) method developed by Brooks and Hughes (1982) is used.

In order to deal with moving free surfaces in surface water modeling, the moving grid method is used in combination with the Arbitrary Lagrangian-Eulerian (ALE) representation (Chan, 1975) of the governing equations. In the ALE representation, arbitrary velocity can be assigned to node movement, thus the grid movement in the interior of the domain is independent of the flow velocity. On the free surface, it is not necessary for the grid node to follow the local velocity as far as the movement of the grid node reflects the deformation of the surface. Therefore, it is possible for the moving grid method to maintain reasonably shaped meshes and describe the free surface boundary accurately at the same time.

Semi-Lagrangian Method: In the presented work, the optional Semi-Lagrangian approach is applied to momentum equations in the surface water model and the thermal and salinity transport equations in both surface water and subsurface media. To apply the semi-Lagrangian method, the backward particle tracking is conducted to find the locations of the target points. Namely for given velocity field at both the current time step and the previous time step, the backward movement of the virtual particles are tracked along their path lines from their locations at the current time step. The change of velocity is taken into account by using bilinear interpolation in both space and time. The particle tracking technique for 3-D quadratic element with moving grid has been developed. In order to improve the accuracy of particle tracking, the 3-D global elements are divided into smaller linear sub-elements, and the backward particle tracking is conducted within each sub- element. Therefore, the particle tracking algorithm is designed for the sub-element, which may have one of the following geometries: hexahedron, triangle-based prism, and tetrahedron. The basic task of 3-D particle tracking within a sub-element is to determine the location of the target point on a target boundary surface for a given source point. The particle tracking algorithm used in this work is a modified version of that found elsewhere (Cheng et al., 1998).

5. COUPLING SURFACE WATER AND GROUNDWATER MODELS

A rigorous coupling that does not introuduce non-physics parameters holds the key to make the integrated surface and groundwater model "truly" physics-based. There are two types of connection between the surface water and groundwater as shown in Figure 1. If the change of media property near the interface of surface water and groundwater can be described (resolved) by the 3-D subsurface mesh, the interface is considered a direct connection. Otherwise, the interface is an indirect connection, such as a thin layer of clay/sediment, which cannot be resolved by a reasonable 3-D subsurface mesh.

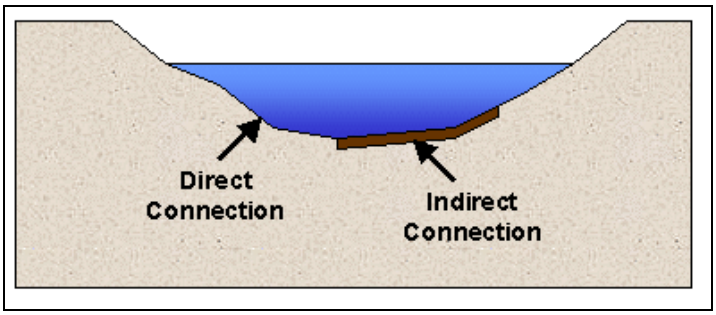

Figure 1 Two types of surface water and groundwater connections

At the interface with direct connection, the fluxes through the interface are obtained without introducing any new parameter by imposing the continuity of fluxes and state variables as:

$$\Phi^S = \Phi^G \quad \text{and} \quad \Psi^S = \Psi^G \tag{17}$$

where Φ^S and Φ^G, respectively, are the fluxes of surface water and groundwater water, respectively, through the interface and Ψ^S and Ψ^G, respectively, are the state variables in surface water and groundwater, respectively. In the case of fluid flow, Φ and Ψ, respectively, represents volumetric flow rate and pressure, respectively. In the case of thermal transport, Φ and Ψ, respectively, represents thermal flux and temperature, respectively. In the case of salt transport, Φ and Ψ, respectively, represents salt flux and salinity, respectively.

At the interface with indirect connection, the fluxes are formulated with a linkage term

$$\Phi^S = \Phi^G \quad \text{and} \quad \Phi^G = f(\Psi^S, \Psi^G; K) \tag{18}$$

where $f(\Psi^S, \Psi^G; K)$ is the linkage term which is a function of Ψ^S, Ψ^G, and K (K represents the material property of the thin layer that makes the surface water and groundwater indirectly connected and is not included in the groundwater discretization). For example, in the case of fluid flow, $f(\Psi^S, \Psi^G; K)$ can be formulated as $f(\Psi^S, \Psi^G; K) = K \times (\Psi^S - \Psi^G)$.

6. PRELIMINARY SIMULATIONS OF FLOW AND SALINITY TRANSPORT IN INTEGRATED LOXAHATCHEE RIVER ESTUARIES AND SUSURFACE MEDIA

The ultimate goal of the presented work is to apply the coupled model for simulating salt water movement in the Loxahatchee River and in groundwater under the influence of tides in the Atlantic Ocean and freshwater input from the upstream tributaries of the river. The calibration and validation of the model are beyond the scope of this paper. Here only a preliminary test run is given to illustrate the successful development of the 3-Dimensional Integrated Surface and Groundwater (3DISG) computational model. Figure 2 shows an aerial picture of the study area overlapped with the top view of the mesh for surface and subsurface domain in the integrated model. In Figure 2 the mesh of surface water model is in blue, the mesh of subsurface domain is in orange.

Figure 2 Aerial picture of the Loxahatchee River and Estuary area with overlapped model mesh for integrated surface and subsurface model

The three-dimension mesh of both the surface and the subsurface domain are generated by stretching the two-dimensional mesh (the base mesh) in Figure 2, along the vertical direction. In the surface water domain, four layers of three-dimensional meshes lay over the base mesh and the grid nodes distributed uniformly in the vertical direction. In the subsurface domain, ten layers of meshes are built from the ground surface and stretched vertically downward. There are ten layers of mesh below the ground surface and six layers below the river bed. The bottom boundary of subsurface domain is set at –50 ft NGVD29. The three-dimensional surface water model includes 5,224 elements and 32,064 nodes with horizontal element size ranging from 3,500 ft in the Atlantic Ocean to 15 ft near the Kitching Creek. The three-dimensional subsurface domain includes 47,280 elements and 50,426 nodes. A perspective view of the three-dimensional mesh of the integrated model is given in Figure 3. Figure 4 gives a closer view of the model mesh near the inlet of the Loxahatchee River.

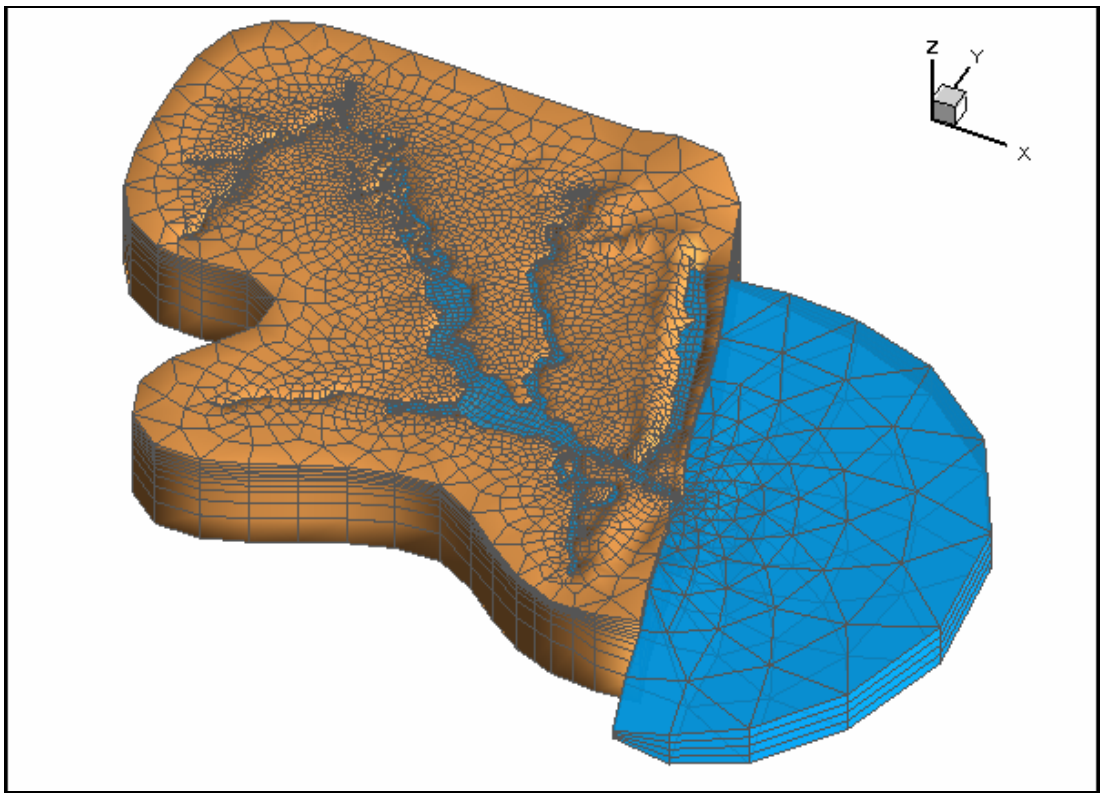

Figure 3 Three-dimensional integrated surface and subsurface model mesh

The purposes of model testing run are 1) to test the flow and salinity transport solvers of the three-dimensional both surface and subsurface models and identify any possible errors in the code development; 2) to test the data structure and tracking algorithm for the interface between the surface and subsurface model; and 3) to test the coupling between the surface and subsurface model.

In the testing run, the realistic boundary conditions for the surface water model, as used in the calibration of the model in a previous study, are sued. For the subsurface model, since the data are not available at this moment, artificial boundary conditions are used. At ground surface (top boundary of the subsurface domain except the river bed) and bottom of the subsurface domain, the zero flux Cauchy condition is used. This implies that the rainfall infiltration rate and the evaporation rate are assumed as zero. On the side boundary of the subsurface domain, except the interface with the surface water body, a constant Dirichlet boundary condition is given for pressure head. The zero flux Neumann boundary condition for salinity is imposed at all boundaries mentioned above. The testing run starts as a cold start with uniform water stage and pressure head in entire domain. Initially, zero salinity is assumed throughout the model domain except at the ocean boundary, where the salinity is 35.5 ppt. It should be pointed out that the integrated model is capable of dealing different types of boundary conditions. Of course, more realistic boundary conditions for the subsurface domain will be used for the model calibration run in the final modeling.

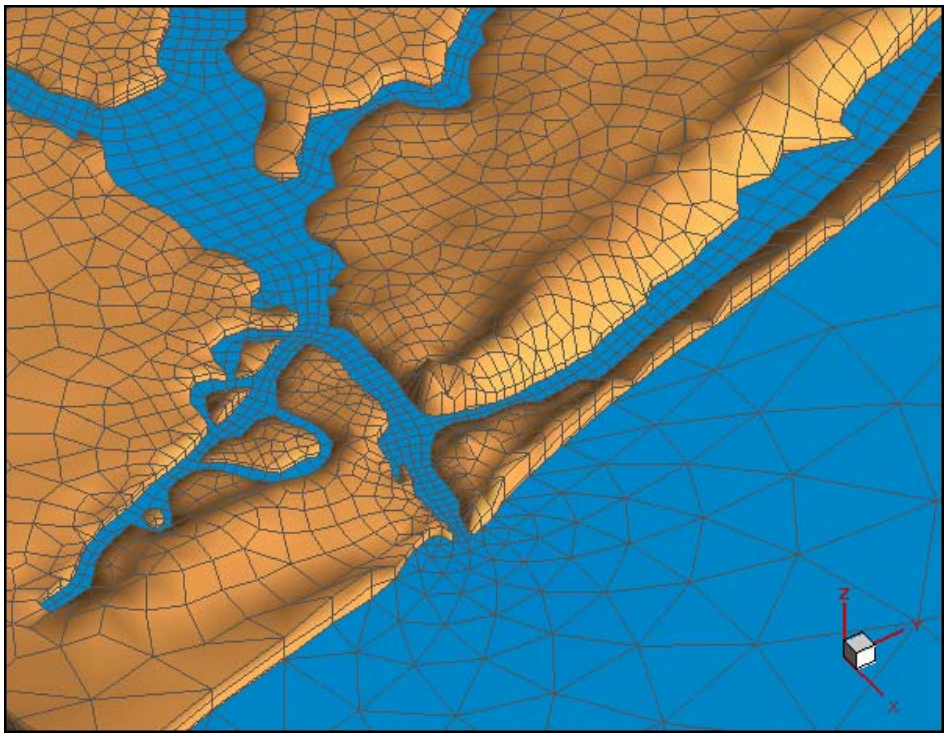

Figure 4 A close view of model mesh near river inlet

Figure 5 shows the distribution of pressure head in the subsurface domain at t = 53 hours from the cold start. In Figure 6, the subsurface pressure head is displayed together with the water elevation in the surface water domain. The distribution of salinity in the river as well as in the subsurface domain can be found in Figure 7.

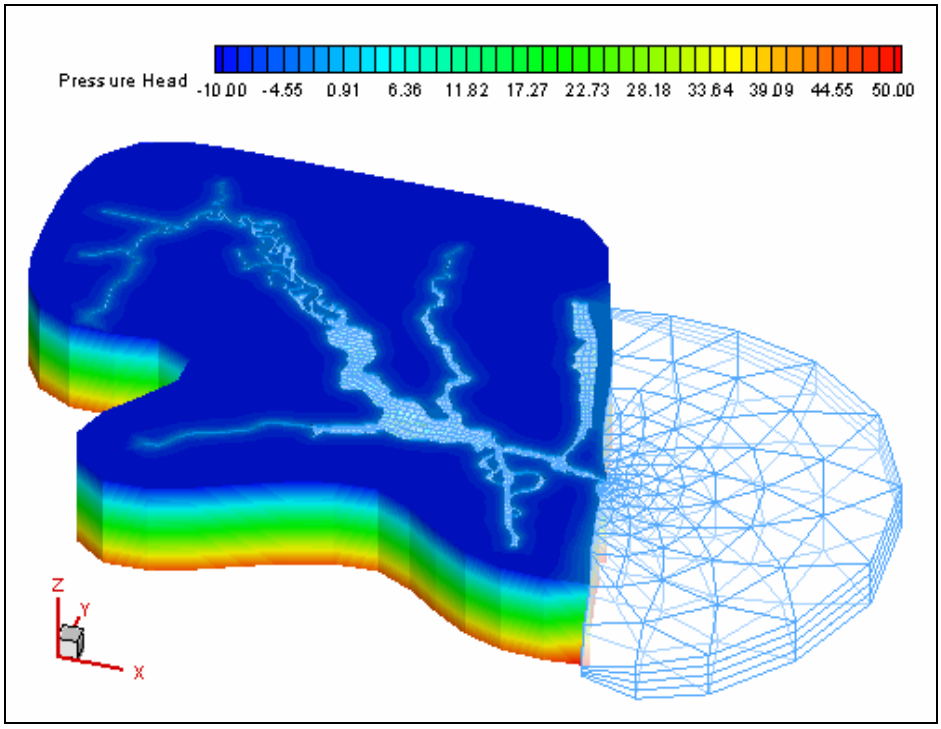

Figure 5 Distribution of pressure head in the subsurface domain at *t* = 53 hours from a cold start

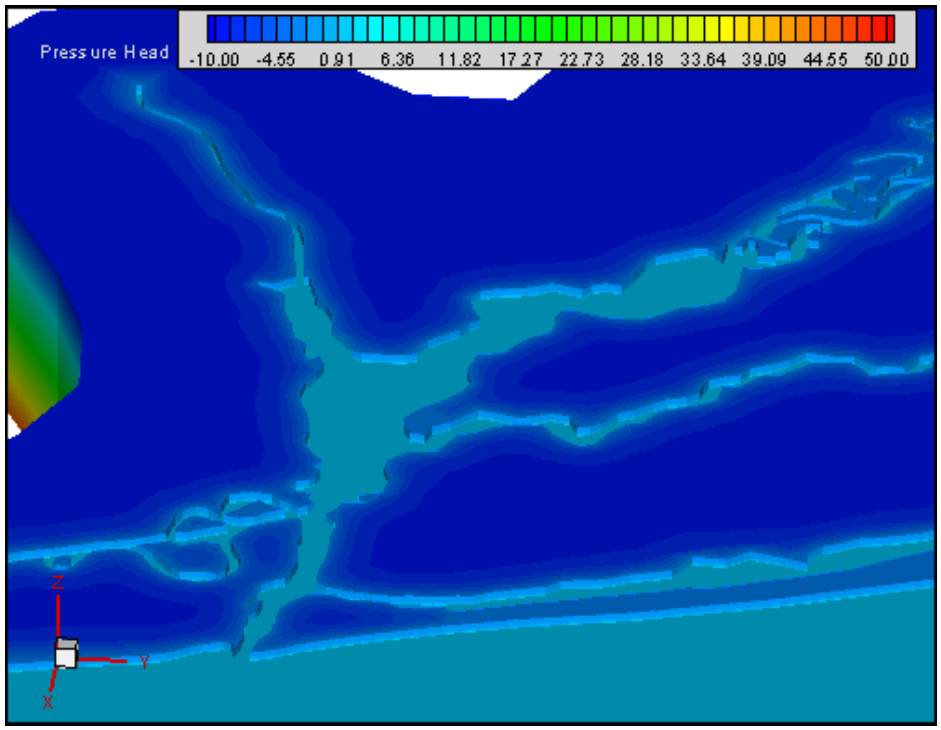

Figure 6 Contours of pressure head in the subsurface domain and water elevation in surface water domain at *t* = 53 hours from a cold start

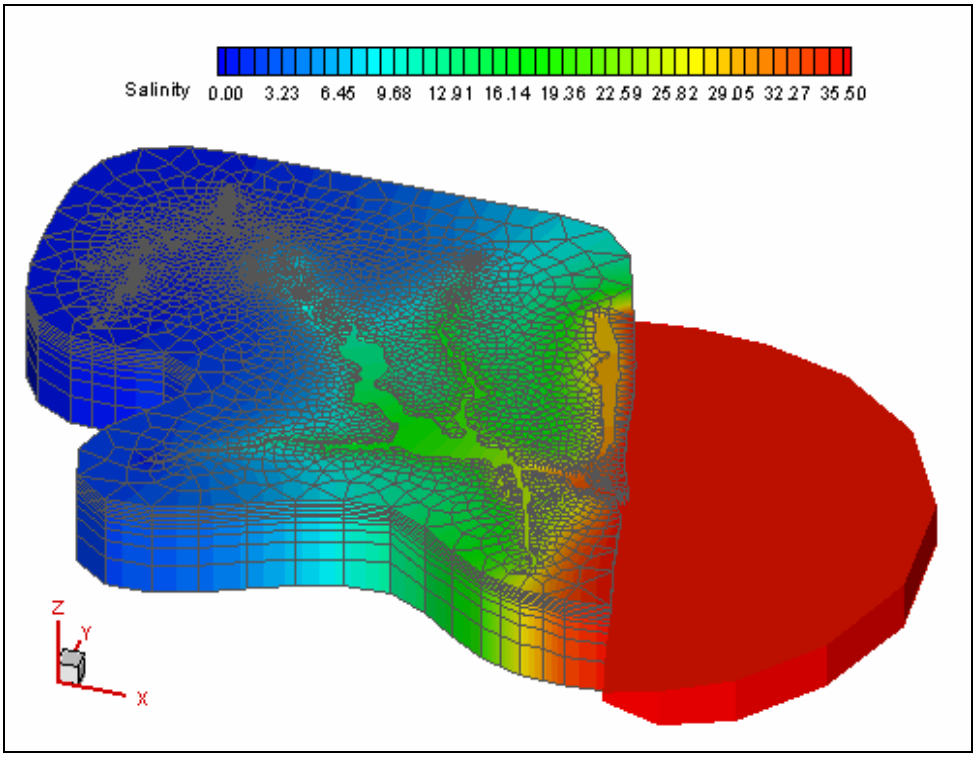

Figure 7 Contours of salinity in the subsurface domain and water elevation in the surface water domain at *t* = 53 hours from a cold start

The simulation from the testing run has indicated that the three-dimensional integrated model runs well and results are reasonable. Our next tasks are 1) Use the actual topological data to determine the ground surface of the model; 2) Collect data from subsurface media to use as the boundary conditions for the finally integrated model.

CONCLUDING REMARKS

A three-dimensional computational model that covers integrated surface water and groundwater domains has been developed. The surface water module was based on Navier-Stokes equations with or without hydrostatic assumption and scalar transport equations of salinity and temperature. The Boussinesq approximation is employed to deal with the buoyancy force due to temperature and salinity variations. The Arbitrary Lagrangian-Eulerian (ALE) representations of the governing equations are combined with the moving grid method to solve surface flow problems involving free surfaces. The subsurface flow module was based on Richards' equations and scalar transport equations of salinity and temperature. The surface water flow and subsurface flow are rigorously coupled via the imposition of the continuity of fluxes and state variables for a direction connection. The flux formulation was used for a non-direct connection. The numerical solution is obtained with finite element methods or a combination of finite element and Semi-Lagrangian (particle tracking) methods. The preliminary test application of the coupled model to the Loxahatchee River shows its capability of solving flow and transport problems in the complex, integrated river/estuary and subsurface media system.

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