Simulations of Ecosystem Hydrological Processes Using a Unified Multi-Scale Model

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Abstract. This paper presents a unified multi-scale model (UMSM) that we developed to simulate hydrological processes in an ecosystem containing both surface water and groundwater. The UMSM approach modifies the Navier-Stokes equation by adding a Darcy force term to formulate a single set of equations to describe fluid momentum and uses a generalized equation to describe fluid mass balance. The advantage of the approach is that the single set of the equations can describe hydrological processes in both surface water and groundwater where different models are traditionally required to simulate fluid flow. This feature of the UMSM significantly facilitates modelling of hydrological processes in ecosystems, especially at locations where soil/sediment may be frequently inundated and drained in response to precipitation, regional hydrological and climate changes. In this paper, the UMSM was benchmarked using WASH123D, a model commonly used for simulating coupled surface water and groundwater flow. Disney Wilderness Preserve (DWP) site at the Kissimmee, Florida, where active field monitoring and measurements are ongoing to understand hydrological and biogeochemical processes, was then used as an example to illustrate the UMSM modelling approach. The simulations results demonstrated that the DWP site is subject to the frequent changes in soil saturation, the geometry and volume of surface water bodies, and groundwater and surface water exchange. All the hydrological phenomena in surface water and groundwater components including inundation and draining, river bank flow, groundwater table change, soil saturation, hydrological interactions between groundwater and surface water, and the migration of surface water and groundwater interfaces can be simultaneously simulated using the UMSM. Overall, the UMSM offers a cross-scale approach that is particularly suitable to simulate coupled surface and ground water flow in ecosystems with strong surface water and groundwater interactions.

*Keywords: multi-scale modelling; computational fluid dynamics; groundwater flow;
groundwater and surface water interactions*

1. Introduction

Fluid dynamic processes govern the spatial and temporal dynamics of soil moisture condition, groundwater and surface water flow, and fluid-carrying mass and energy exchange and cycling in ecosystems. Fluid flows affect the dynamics of biogeochemical processes, especially in the Earth's critical zones (Chorover et al. 2007) such as active groundwater and surface water interaction areas where microbial activities are affected by frequent groundwater and surface water exchange that controls organic carbon and nutrient supplies for microbial growth and survival, and by sediment and soil inundation and draining that change saturation and redox conditions influencing microbial respiration and its products (Mitsch and Gosselink 2000, Cherry 2011). Active groundwater and surface water interaction zones, such as wetlands, are important sources and sinks in global cycling of carbon and nitrogen; in retarding and degrading metals and organic contaminants; and in producing and mitigating greenhouse gases (Winter et al. 1998).

Various models have been developed to mathematically represent fluid flow processes in ecosystems. These models typically separate an ecosystem into groundwater and surface water components where different physical laws and mathematical equations are required to describe the momentum and mass conservation of fluid. These mathematical equations are then coupled at the groundwater and surface water interfaces using various coupling approaches (Morita and Yen, 2000, 2002, Furman, 2008, Jolly et al. 2008, Ebel et al. 2009). Generally, these coupling approaches can be divided into two groups: 1) assuming that the momentum and mass exchange

between surface water and groundwater can be described using the 1st-order mass exchange (e.g., Panday and Huyakorn 2004, Ebel et al. 2009), and 2) enforcing the continuity of pressure and flux cross the interfaces (e.g., Kollet and Maxwell 2006, Maxwell and Kollet 2008, Maxwell 2009). In these coupling approaches, surface water flow is typically described using two dimension equations, such as Saint-Venant-like equations (Morita and Yen, 2002, Furman, 2008), which can be derived by depth-averaging three-dimensional Navier-Stokes (N-S) equations. The groundwater flow is commonly described using three dimensional Darcy law and mass conservation equations. These coupling approaches require iterations at the interfaces for numerical convergence and accuracy (Bronstert et al. 2005, Gossel 2011). The iteration can become a challenging problem when simulating coupled water flow in active groundwater and surface water interaction zones where interaction interfaces may frequently migrate as ground surface is inundated and drained. Modeling approaches that consider groundwater and surface water as an integrated system are needed to simulate hydrological processes in ecosystems.

In this paper, we report a unified multi-scale model (UMSM) to simulate coupled surface water and groundwater flow in ecosystems. The UMSM merges the Navier-Stokes (N-S) equation with the Darcy law into a single equation to describe fluid momentum, and uses a generalized equation to describe fluid mass conservation under both saturated and unsaturated conditions. Numerically, the UMSM becomes the N-S equation in surface water, and becomes the Darcy law in subsurface. Using the N-S equations to describe surface flow avoids averaging and simplification in numerical treatment of surface flows. The UMSM was first proposed and successfully demonstrated to describe pore-scale fluid flow in soils containing mixed pores and porous media where fluid flow in pores follows the N-S equation and in porous media follows the Darcy law (Yang et al. 2014). In the previous study, we speculated, by analogue, that the

UMSM would also be able to simulate hydrological processes in ecosystems by treating surface water bodies as pores and subsurface as porous media. Here we demonstrated that it can indeed do so. The advantage of the approach is that the same set of equations can simulate groundwater and surface water flow so that the ecosystem can be treated as an integrated model system.

2. Theory and Model

The fluid momentum in the UMSM is described by merging the N-S equation and Darcy law into a single equation (Yang et al. 2014):

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -g \nabla h + \nu \nabla^2 \mathbf{u} + \mathbf{g} - g \mathbf{K}^{-1} \cdot \mathbf{u} \quad [1]$$

where $\mathbf{u}$ is the velocity vector, t is the time, g is the gravitational constant, $\mathbf{g}$ is the gravitational force, h is the pressure or water head, ν is the effective kinematic viscosity ($\nu = \mu / \rho$, where μ is the dynamic viscosity and ρ is the fluid density), and $\mathbf{K}^{-1}$ is the matrix inverse of the hydraulic conductivity tensor. The last term in the right hand side of Eq. [1] is the Darcy force term, which distinguishes the UMSM from the classic N-S equation. Eq. [1] becomes the N-S equation for surface water domain when the Darcy force term is ignored by setting a large, constant numerical value for the diagonal elements in tensor $\mathbf{K}$ (Yang et al. 2014). Eq. [1] becomes the Darcy law in porous media when the acceleration terms (left side) and viscous term (second term of the right side) become negligible (Popov et al. 2009, Yang et al. 2014).

The mass conservation equation in the UMSM is generally described using the following equation, (Yeh 1999):

$$F \frac{\partial h}{\partial t} = -\nabla \cdot \mathbf{u} + s \quad [2]$$

where s is the source/sink term, and F is the generalized storage coefficient. The storage coefficient in Eq. [2] is defined as:

$$F = \alpha' \frac{\theta}{n_e} + \beta' \theta + n_e \frac{dS}{dh} \quad [3]$$

in which n_e is the effective porosity, S is the degree of effective saturation of water, θ is the effective soil moisture content, α' is the modified compressibility of the soil matrix, and β' is the modified liquid compressibility. The degree of effective saturation of water may be described using various constitutive models to link saturation degree with hydraulic pressure (Tuli and Hopmans 2004). For the demonstrative purpose, the van Genuchten model was used in this study (Gulbransen et al. 2009, Ghanbarian-Alavijeh et al. 2010):

$$S_e = \frac{S - S_m}{1 - S_m} = \left(1 + (\alpha|h|)^n\right)^{-m} \quad [4]$$

$$K = K_s S_e^{1/2} \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \quad [5]$$

where S_e is the effective saturation, K is the hydraulic conductivity under unsaturated condition, S_m , α , n , and $m = 1 - 1/n$ are the empirical parameters, and K_s is the hydraulic conductivity under saturated condition.

Eqs. [1-5] are the complete set of equations for the U MSM. It becomes a traditional groundwater flow model when the fluid momentum equation (Eq. [1]) is replaced by the Darcy law. Eqs (1) is discretized using a semi-implicit scheme, and Eq 2 is discretized implicitly:

$$\left(1 + g\mathbf{K}^{-1}\Delta t\right)\mathbf{u}^{n+1} = -g\Delta t\nabla h^{n+1} + \mathbf{u}^n + \Delta t\left(\mathbf{g} + \nu\nabla^2\mathbf{u}^n - \mathbf{u}^n \cdot \nabla\mathbf{u}^n\right) \quad (6)$$

$$F^{n+1}(h^{n+1} - h^n) = \Delta t\left(\nabla \cdot \mathbf{u}^{n+1}\right) + s^{n+1} \quad (7)$$

where n is the current time step, and $n+1$ is the next time step. The semi-implicit momentum equation (Eq. 6) is spatially discretized using a staggered Cartesian grid, in which the 2nd-order

Adams–Bashforth scheme is used for the advection term ($\mathbf{u}^n \cdot \nabla \mathbf{u}^n$), and central differencing is used for the diffusion term $\nabla^2 \mathbf{u}^n$ (Ferziger and Peric, 2001). SIMPLE algorithm is used for solving Eqs 1 and 2 (Patankar, 1980). In each time step, the pressure and velocity estimated from last iteration step is used to solve the momentum equation (Eq. 6) for the next step velocity, which is then used to update pressure (Eq. 7). The updated pressure is used to calculate generalized storage coefficient (Eq. 3) and hydraulic conductivity (Eqs 4 and 5) if in unsaturated numerical nodes, which are then used to solve Eqs. 6 and 7 again. This process is iterated until convergence with a convergence criterion of 10^{-6} on the sum of absolute residuals of the local mass balance equation as defined by Patankar (1980).

The numerical scheme is stable because of the implicit scheme used for solving the mass conservation equation (Eq. 7) (Press et al., 1992). Courant-Friedrichs-Lewy (CFL) condition is used in selecting time step. The time step calculated from the CFL condition is, however, for explicit numerical scheme. Numerical tests for the examples as presented in the later sections indicated that the semi-implicit numerical scheme is stable using a much larger time step, for example, 10 times of the CFL time step. The computational efficiency of the UMSM is close to that for solving a typical groundwater flow problem in unsaturated porous media using the Darcy law models because of the explicit nature for calculating flow velocity (Eq. 6). More details of the numerical procedures can be found elsewhere (Yang et al. 2014).

3. Results and Discussion

3.1 Model Comparison for Groundwater Simulations

The UMSM approach has been verified previously using various water flow cases in mixed media containing pores and porous domains (Yang et al. 2014). The applicability of the

UMSM in surface water can be demonstrated by setting a large value for each diagonal element in K tensor so that the Darcy force term in Eq. [1] becomes negligible as compared to other terms, and Eq [1] becomes that N-S equation. To evaluate the applicability of the UMSM to describe groundwater flow, a hypothetical, two dimensional case was designed (Fig. 1). The computational domain (L= 120 m, H = 30 m) consists of an aquifer with groundwater in exchange with surface water in the nearby stream. Only the left side of the stream was shown in Fig. 1 assuming that the right side is symmetric for the demonstrative purpose. For this specific case, the saturated hydraulic conductivity in the aquifer (Fig. 1) was calculated from porosity, which was assumed randomly distributed, using the following equation (Bear, 1972):

$$K_s = \frac{n_e^3}{(1-n_e)^2} \cdot \frac{g}{5M_s^2\nu} \quad [8]$$

where M_s is the specific surface area of solid grains with respect to solid volume. Parameters for silt loam from literature (Schaap & Leij 1998; Zhu & Mohanty 2002) were used in calculating hydraulic conductivity under unsaturated conditions using Eq. [8] (i.e., $S_m = 0.16$, $\alpha = 2 \text{ m}^{-1}$, $n = 1.4$).

Two cases of model simulations were compared for this example. One uses the UMSM to simultaneously simulate groundwater and surface water flow, as well as the associated inundation and draining of river bank (Fig. 1). The left, right, and bottom boundaries were assumed to be no flux boundaries. Infiltration was hypothetically imposed at the highest location at the left side that is far away from the surface water (Fig. 1). Other upper boundary conditions were not fixed, but determined by solving Eqs. [1-5]. The initial condition in the aquifer was generated by solving the UMSM assuming no infiltration, and a steady state surface water table ($y/H = 0.25$, right side), and a steady state groundwater water table at the left boundary ($y/H = 0.8$).

Fig. 1 A computational domain containing both aquifer and surface water (river) for evaluating the UMSM. Only left side of the river was shown. The right side was assumed to be symmetric to the left side. The colour denotes the saturated hydraulic conductivity in the aquifer.

The other case is to use a traditional method (i.e., using Darcy law to replace Eq. [1], and keeping other equations the same) to simulate groundwater flow by imposing a pressure boundary condition at the surface water and groundwater interface. The traditional method, however, cannot simulate surface water table change. Consequently, the simulated change in surface water table from the UMSM was used as the pressure boundary condition at the groundwater and surface water interface in this case. The upper boundary conditions were not fixed, but determined by solving Eqs. [1-5] with Eq. (1) replaced by the Darcy law. All other boundary conditions are the same as for the first case (i.e., the case using the UMSM). The initial condition in the aquifer was generated by solving the Darcy law-based equations assuming the same infiltration and boundary conditions described above for the UMSM case.

Fig. 2a showed that the simulated initial steady state condition using both the UMSM and Darcy law-based equations was the same, confirming that Eq. [1] became the Darcy law in the aquifer. Fig. 2b shows a snapshot of water distribution and water flow streamlines in both aquifer and surface water domain generated by the UMSM after 320 hours of simulations superimposed

on the initial condition (Fig. 2a). The streamlines show water flow from left/top toward right/bottom as a result of infiltration at the left side. The steady rate of infiltration was 0.1m/hr in the entire simulation period. The streamlines penetrate the groundwater and surface water interface, causing the rise of surface water table. The variable water saturation degree and complex streamline shapes were caused by heterogeneous distribution of hydraulic conductivity (Fig. 1). The simulated groundwater table in Fig. 2b was lower than the initial water table (Fig. 2a). This is because a fixed, but a high ($y/H = 0.8$) water table condition was imposed at the left side in generating the initial condition. This fixed water table condition was eliminated when simulating water flow under infiltration condition.

Fig. 2c shows a snapshot of water distribution and water flow streamlines generated in the second case using the traditional, Darcy law-based approach. In the simulations, temporal change in surface water table and the coverage of river bank by the surface water simulated from the UMSM (Fig. 2b) was used to impose boundary pressure condition for the aquifer. The water distribution and streamlines simulated using the Darcy law-based approach were generally consistent with those from the UMSM (Figs. 2b and 2c) because the momentum equation (Eq. [1]) becomes the Darcy's law in the aquifer. Slight difference existed, however, because the UMSM implicitly imposed the continuity of both pressure and flux, while the Darcy law-based model only imposed the pressure condition at the surface water and groundwater interface. Nevertheless, the differences were small, and both methods generated almost identical results. Using the UMSM, however, the spatiotemporal change in surface water table can be simultaneously simulated.

Fig. 2 Simulated water saturation degree and flow streamlines in a 2-dimensional system containing an aquifer and surface water body: a) initial condition of water distribution simulated using both UMSM and Darcy-law based approach; b) a snapshot of the water distribution and flow streamlines at time ($t = 320\text{hr}$) generated by the UMSM under the infiltration condition; and c) water distribution and streamlines generated using the Darcy law-based approach.

3.2 Model Comparison for Coupled Groundwater and Surface Water Flow

The UMSM is further tested by comparing with WASH123D, a first-principle, physics-based models for simulating coupled surface water and groundwater flow. The WASH123D is

a model that uses different mathematical equations to describe surface water and groundwater flow, and then couples them at their interfaces (Yeh et al., 2006). The model can simulate processes of infiltration, evapotranspiration, recharge, moisture redistribution in vadose zone, groundwater flow, surface runoff, and river/stream. WASH123D treats river flow as one dimensional system, overbank flow as two dimensional system, and groundwater as three dimensional system. The WASH123D is a community code for both groundwater and surface water community.

A benchmark problem was constructed that consists of a stream passing through an underlying unconfined aquifer (Fig. 3a). The size of the aquifer is 900 m $\times$ 900 m $\times$ 50 m. The stream is located near the center of the domain ($x = 500$ m). The upstream of the stream is at $y = 900$ m. The saturated hydraulic conductivity of the aquifer is assumed to be $K_x = 10^{-4}$ m/s, $K_y = 10^{-5}$ m/s and $K_z = 5.0 \times 10^{-6}$ m/s. The effective porosity is 0.3. The unsaturated characteristics for the aquifer are linear functions of pressure head (Table 1). The aquifer is discretized into 9 $\times$ 9 $\times$ 10 non-uniform grid cells (Fig. 3a). The stream is 900 m long, and has a bottom slope of 5/1,000. Its cross-section is rectangular, with a width of 10 m. The Manning's coefficient is 0.03. The stream is divided into 9 segments (numerical grid cells) in y-direction that are corresponding to the underlying numerical grid cells in the aquifer. Initial and boundary conditions for both aquifer and stream are shown in Table 2.

Table 1. Unsaturated characteristics

Pressure Head (m)	Moisture Content	Relative Hydraulic Conductivity	Index of Water Capacity
-100000	0.15	0	0
-100.0001	0.15	0	0
-100	0.15	0	1.5e-3
0	0.3	1	1.5e-3
0.0001	0.3	1	0
100000	0.3	1	0

Figure 3. An example of coupled groundwater and surface water flow. Plot a: modelling domain consisting of river (line), overbank flow domain, and unconfined aquifer; plot b: stream flow rate at the upstream boundary; plot c: rating curve at the downstream boundary; plot d: snapshot of simulated pressure head distribution at simulation time of 14200 seconds; and plot e: simulated pressure head using both WASH123D (lines) and UMSM (symbols) along z (depth) direction at $x = 400\text{m}$ and $y = 500\text{m}$.

Table 2. Initial and boundary conditions for the aquifer and stream

	Initial Condition	Boundary Condition
Aquifer	Total head = 25 m	Dirichlet (total head of 25 m) on the bottom 3 layers at surface of $y=0$ m and $y = 900$ m; Zero flux condition at the top; Other boundaries: impermeable.
Stream	Dry	An inflow hydrograph (Fig. 3b) is applied at the upstream end of the stream ($y = 900$ m); A discharge rating curve (Fig. 3c) is applied at the stream outlet ($y = 0$ m).

Figure 3d shows a snapshot of the simulated pressure head distribution at a simulation time of 14200 s using the WASH123D. The simulated results from the UMSM are overlapped with those from WASH123D, and consequently are not provided. Figure 3e shows the comparison of simulated water pressure head (m) as a function of depth at location of $x = 400$ m, and $y = 500$ m. The results show that simulated water pressure from the UMSM is nearly identical to those from the WASH123D. The CPU time for this specific case is less than 2 seconds for both UMSM and WASH123D on a Dell desktop workstation with 12 CPU cores and 3.47GHz for each core. The WASH123 used slightly less CUP time (1.7 seconds) than the UMSM (1.8 seconds).

3.3 Simulation of Hydrological Processes at DWP site

The DWP site, an 4,654 ha preserve (including 1416 ha wetland) located at the Northern Greater Everglades Watershed, plays an important role in maintaining the ecosystem balance within the upper Reedy Creek Basin in central Florida (Fig. 4a). The site is relatively level with an average elevation approximately 18 m above sea level. The vegetation is dominated by long leaf pine flatwoods in the northern portion, slash pine flatwoods on the southern portion with scattered wetland including both woody and graminoid vegetation. The DWP site was classified as a mitigation site in early 1990s for wetland disturbance by the Walt Disney World

Corporation and the Greater Orlando Aviation Authority. It has undergone extensive hydrological/vegetation restoration consisting of filling in drainage canals and reestablishing a normal fire regime (Drake and Weishampel 2001).

3.3.1 Hydrological Properties

Hydrological characteristics of the Reedy Creek Basin, which includes the DWP site (Fig. 4a), have been well documented elsewhere (Ali 1999). Briefly, the DWP site receives inflow from the upstream Reedy Creek with inflow rates seasonally variable and regulated by water management measures in the basin. The surface water flow disperses inflow velocity and direction after entering the site due to the flat terrain at the DWP site. There are 11 monitoring stations monthly measuring surface water stage and flux in the Reedy Creek Basin. Among these monitoring stations, Highway 101 station, which is located at the intersection of State Highway 101 and Reedy Creek, is near the north boundary of the modeling domain. Consequently, in this study, the monitored surface water flux data at the Highway 101 station were used as the surface water inflow boundary condition at the north side of the DWP site (Fig. 4). The inflow flux varied significantly (Fig. 4b) in response to upstream flow and precipitation (Fig. 4c). The inflow flux apparently also affected by the regional water management as the change in inflow flux deviates from the timing of precipitation.

The DWP site is characterized by a humid subtropical climate with occasional extremes of temperature and precipitation. Average monthly precipitation is 107 mm (Fig. 4c), much of which (85 %) occurs during the months from June to September. The soils at the site are dominated by fine sand and silt, and frequently inundated in response to precipitation and upstream flow at the Reedy Creek Basin.

Fig. 4 (a) DWP site (red line), sub-basin boundaries (purple line), computational domain (black line), and elevation contour of ground surface (color legend); (b) monthly variation in river discharge at the Florida Highway 101 monitoring station (denoted as inflow location in plot a) along the Reedy Creek stream; and (c) monthly statistics of rainfall in the Reedy Creek Basin.

3.3.2 Computational Domain and Discretization

The computational domain was selected along the boundary lines of sub-basin in the Reedy Creek watershed (black lines in Fig. 4a) so that a simplified boundary condition (no-flux conditions) may be applied along most part of the computational domain boundaries. The computation domain contains one inflow flux boundary at the north (Fig. 4a). The median monthly variation in flow rates at the Highway 101 station (Fig. 4b) was directly used as the inflow boundary condition for surface water flow. There are two surface flow outlets at downstream connecting Lake Cypress and Lake Hatchineha (Fig. 4a). Lake Russell at the north was entirely included in the computational domain.

A high resolution digital elevation map (DEM) was used in this study to delineate the sub-basin boundary, and to discretize the numerical domain. The DEM provides topographic information for the delineation of sub-basins. It was downloaded from the National Elevation Dataset (NED) website of U.S. Geologic Survey (USGS) at the one-third-arc-second resolution and converted to the projection of USA Contiguous Albers Equal Area Conic USGS version. The size of each resulting grid cell is about 11m x 11m x 1m along x, y, z directions, respectively. The entire computational domain consists of $1200 \times 1600 \times 22 = 4.2 \times 10^7$ grid cells in this 234 km² area. The DEM data was processed using ArcGIS (©Esri) and its toolbox then exported as ASCII file including the coordinates of the grid cells. The horizontal (x, y) and vertical (z) coordinates of each grid cell are then extracted from the DEM data and directly read into the UMSM as computational grid cells. For this specific site, the land surface topography was located in the vertical coordinates with $z=14 - 22$ m, Fig. 5a. The numerical cells from $z = 0$ to 14 m was below groundwater surface.

The same parameters for the unsaturated silt loam as used for simulations in Fig. 2 were used to calculate unsaturated hydraulic conductivity (Eqs. [4-5]). The porosity was randomly generated in soils with a mean of 0.32, and maximum of 0.5, which was then used to calculate saturated hydraulic conductivity using Eq. [8]. The model considers precipitation, inflow from north, and outflow at the south. Evaporation and transpiration were not considered in the simulation, but can be included if needed through the source and sink term in Eq. [2].

3.3.3 Model Simulation Results

Model simulations using the UMSM were run continuously for 18 years with the same yearly variations in inflow rate (Fig. 4b) and precipitation (Fig. 4c). An arbitrary zero flow velocity field was assumed for the initial condition because of unknown nature of water distribution and flow velocity at the site. After 18 years of simulations, dynamic steady state in flow velocity, water stage, and saturation condition in both surface water and groundwater was reached. The dynamic steady state results were used for further analysis of hydrological processes at the site.

The simulated monthly snapshots of water distribution and saturation (Fig. 5) show the dynamic variation in surface water coverage and soil saturation condition at the site. The area of surface water coverage was broader from October to February, and became smaller in summer months June - August, primarily reflecting the influence of inflow (Fig. 4b) with about one month lag period. Local precipitation was, however, higher during the summer months, suggesting that the effect of local precipitation was less than that from the upstream inflow. While the simulated water distribution was generally consistent with the measured data in the Reedy Creek basin (Ali 1999), we noted that the simulation results depended strongly on the historical water stage at the highway 101 station, which was the only monitored data used in the

378 simulations as the boundary condition. Potential error in the monitoring data (Ali 1999) would
379 alter the simulation results. Nevertheless, the results in Fig. 5 showed that the UMSM can
380 simultaneously simulate hydrological processes in ecosystems containing groundwater and
381 surface water. In particular, the expansion and shrinkage of surface water coverage, as well as
382 associated surface water flow such as stream and bank flows, which are important to understand
383 inundation and draining, and their effect on biogeochemical processes in ecosystems, can be
384 simulated without a need of special numerical treatments at the surface water and groundwater
385 interfaces. Traditional methods that use separate models for surface water and groundwater will
386 require time-consuming iterations at their interfaces to simulate interface migration.

Fig. 5 Monthly snapshots of simulated water saturation and distribution at the dynamic steady state at the DWP site. The blue area are occupied by surface water.

The simulated water table depth varied spatially across the simulated domain (Fig. 6).

The water table depth was plotted as the relative distance of water table from local ground

surface. A positive number indicates that the water table is above ground surface, and negative number indicates below ground surface. Fig. 6 shows temporal water table change at 4 locations marked as A, B, C, and D (Fig. 4a). Location A is at north, where water table significantly varied monthly and was always below ground surface (Fig. 6) because of a high elevation. Location B is at the model domain outlet, where water table only slightly varied monthly and was always above ground surface because it was buffered by the surface water in the nearby Lake Hatchineha. Location C is in Lake Russell where water table was always above ground, but varied more than that at location B. The larger variation in water table in Lake Russell was caused by its small reservoir volume that had a less capacity to buffer a large variation in inflow flux from the upstream (Fig. 4b). Location D is in the middle of the model domain (Fig. 4a) where simulated water table was either below or above the ground, depending on season. Location D represents a significant portion of the modeling domain where soils was subject to frequent inundation and draining during high and low surface water seasons, respectively. The monthly change in water table depth is similar at all locations, reflecting the overall changes in water table at the site (Fig. 5). There are no historical observations within the model domain that can be used to directly compare with the model results. Ongoing efforts of biogeochemical and hydrological measurements at the site will provide data in future for validating the model and refining model parameters. In this regard, the simulated variation in water table at different locations at the site (Figs. 5 and 6) may provide a guidance for developing a monitoring network to monitor hydrological processes at the site.

Fig. 6 Simulated monthly change in water table at different locations (A, B, C and D, see Fig. 4a). Water table depth denotes a relative distance from local groundwater surface. A positive number indicates that water table is above ground surface, and a negative number indicates below ground surface.

The magnitude and direction of groundwater and surface water exchange flux varied significantly at the site (Fig. 7). The exchange flux was calculated from the volume change in groundwater part using the following equations:

$$Flux_{exchange} = -\Delta V_{GW} + \Delta P + \Delta Q \quad [7]$$

where ΔV_{GW} is the groundwater volume change, ΔP is the amount of groundwater directly supplied from the precipitation, and ΔQ is the net volume of groundwater flow into the simulation domain through the domain boundaries (i.e., inflow and outflow boundaries). The positive number indicates groundwater discharge to surface water, negative number indicates

surface supplies to groundwater. The exchange flux in Fig. 7 was normalized to the absolute value of the largest exchange flux at the site, which occurred in September and October when surface water supplied to groundwater. The exchange flux varied in response to upstream flow (Fig. 4b) and local precipitation (Fig. 4c), as well as hydrological conditions in the simulation domain. Generally, in the summer season groundwater supplies to surface water due to lower surface water table (Fig. 5); while in the winter season, surface water supplies back to groundwater as surface water table at high levels.

Fig. 7 Normalized exchange flux between groundwater and surface water. A positive number denotes water flux from subsurface to surface, and negative number denotes water flux from surface water to groundwater.

4. Conclusions

In this study, we demonstrated that the UMSM can be used to simultaneously simulate surface water and groundwater flows in ecosystems. The advantage of the UMSM is that the same set of mathematical equations (Eqs. [1-5]) can be applied in both surface water and groundwater. This feature of the UMSM can significantly simplify the procedures of simulating hydrological processes in ecosystems because numerical treatments and iterations at interfacial boundaries between groundwater and surface water are eliminated. Conserving fluid momentum and mass flux across the interfaces between surface water and groundwater is a major challenge in traditional methods using different models for surface water and groundwater flow. This challenge is especially difficult to overcome in wetland, where the interfacial boundaries may frequently change with time. Using a single set of equations, the UMSM automatically conserves the mass and momentum across all simulation domains, making the model an integrated approach for simulating hydrological processes in ecosystems.

Another advantage of the UMSM is that it can be applied at multiple scales from the pore to ecosystem. At the pore scale, the UMSM becomes the N-S equation so that fundamental hydrological processes can be evaluated. When the scale of a simulation domain increases to include both pore and porous media, the USMS becomes the N-S equation in the pore domain, and the Darcy law in the porous domain (Yang et al., 2014). When the scale of a simulation domain increases further to include an aquifer, the UMSM becomes the Darcy law-based model; and eventually when the domain size moves up to the ecosystem scale, the model becomes the N-S equation in the surface water and the Darcy law-based model in groundwater as demonstrated in this study. This multi-scale feature of the UMSM provides an efficient way to

integrate hydrological processes cross scales and cross hydrological domains that are traditionally handled using different models.

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Figure caption:

Figure 1. A computational domain containing both aquifer and surface water (stream) for evaluating the UMSM. Only left side of the stream was shown. The right side was assumed to be symmetric to the left side. The colour denotes the saturated hydraulic conductivity (m/s) in the aquifer.

Figure 2. Simulated water saturation degree and flow streamlines in a 2-dimensional system containing an aquifer and surface water body: a) initial condition of water distribution simulated using both UMSM and Darcy-law based approach; b) a snapshot of the water distribution and flow streamlines at time ($t = 320\text{hr}$) generated by the UMSM under the infiltration condition; and c) water distribution and streamlines generated using the Darcy law-based approach.

Figure 3. An example of coupled groundwater and surface water flow. Plot a: modelling domain consisting of river (line), overbank flow domain, and unconfined aquifer; plot b: stream flow rate

at the upstream boundary; plot c: rating curve at the downstream boundary; plot d: snapshot of simulated pressure head distribution at simulation time of 14200 seconds; and plot e: simulated pressure head using both WASH123D (lines) and UMSM (symbols) along z (depth) direction at $x = 400\text{m}$ and $y = 500\text{m}$.

Figure 4. (a) DWP site (red line), sub-basin boundaries (purple line), computational domain (black line), and elevation contour of ground surface (color legend); (b) monthly variation in river discharge at the Florida Highway 101 monitoring station (denoted as inflow location in plot a) along Reedy Creek; and (c) monthly statistics of rainfall in the Reedy Creek Basin.

Figure 5. Monthly snapshots of simulated water saturation and distribution at the dynamic steady state at the DWP site. The blue area are occupied by surface water.

Figure 6. Simulated monthly change in water table at different locations (A, B, C and D, see Fig. 4a). Water table depth denotes a relative distance from local groundwater surface. A positive number indicates that water table is above ground surface, and a negative number indicates below ground surface.

Figure 7. Normalized exchange flux between groundwater and surface water. A positive number denotes water flux from subsurface to surface, and negative number denotes water flux from surface water to groundwater.