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Simulations of ecosystem hydrological processes using a unified multi-scale model

Xiaofan Yang[a], Chongxuan Liu[a,*], Yilin Fang[a], Ross Hinkle[b], Hong-Yi Li[a], Vanessa Bailey[a], Ben Bond-Lamberty[a]

[a] Pacific Northwest National Laboratory, Richland, WA 99352, USA
[b] University of Central Florida, Orlando, FL 32816, USA

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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.

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., 1999).

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

* Corresponding author at: 3335 Innovation Street, Richland, WA 99354, USA. Tel.: +1 509 371 6350.
E-mail address: Chongxuan.Liu@pnnl.gov (C. Liu).

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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) equation. The groundwater flow is commonly descried 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 mergers the 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):

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

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 ($\nu = \mu/r$, where μ is the dynamic viscosity and ρ is the fluid density), and 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 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):

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

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

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

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):

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

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

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 UMSM. It becomes a traditional groundwater flow model when the fluid momentum equation (Eq. (1)) is replaced by the Darcy law. Eq. (1) is discretized using a semi-implicit scheme, and Eq. (2) is discretized implicitly:

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

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

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. (6) and (7) (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