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Coupling methodology and application of a fully integrated model for contaminant transport in the subsurface system

Yan Zhu [a,b], Liangsheng Shi [a], Jinzhong Yang [a], Jingwei Wu [a,*], Deqiang Mao [c]

[a] State Key Laboratory of Water Resources and Hydropower Engineering Science, Wuhan University, Wuhan 430072, China
[b] Earth and Environmental Sciences, University of Waterloo, Waterloo N2L 3G1, Ontario, Canada
[c] Department of Hydrology and Water Resources, University of Arizona, Tucson, AZ 85721, USA

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SUMMARY

An efficient integrated modeling approach is developed to simulate the contaminant transport in the subsurface system. The unsaturated zone is divided into a number of horizontal sub-areas according to the atmospheric boundary conditions, land use types and hydrological conditions. Solute migration through the unsaturated zone of each sub-area is assumed to be vertical and can be represented by the one-dimensional advection–dispersion equation, which is then coupled to the three-dimensional advection–dispersion equation representing the subsequent groundwater transport. The finite element method is adopted to discretize the vertical solute equation, while the hybrid finite element and finite difference method is used to discretize the three-dimensional saturated solute transport equation, which is split into the horizontal and vertical equations based on the concept of the horizontal/vertical splitting. The unsaturated and saturated solute transport equations are combined into a unified matrix by the mass balance analysis for the adjacent nodes located at the one-dimensional soil column and at the water table. Two hypothetical cases and two field cases are simulated to test the validity of the model with the results compared with those from HYDRUS-1D, SWMS2D and the measured data. The limitations of the model are discussed as well. The analysis of the four cases demonstrates that the proposed model can calculate the water flow and solute transport reasonably even with complex boundary and variable topography conditions. It also shows that the model is efficient to simulate the water flow and solute transport in regional-scale areas with small computational costs. However, the model will lose accuracy when the lateral dispersion effect is dominant in the unsaturated zone.

1. Introduction

Prediction of the contaminant fate is a fundamental work for the remediation of contaminated sites. Thus a reliable and efficient simulation tool is needed (Barry, 1992; Radu et al., 2011). Many models, including analytical models, semi-analytical models and numerical models, have been developed and widely used to describe the water flow, solute transport and even the complex physicochemical processes in the subsurface system (Elrick et al., 1994; Diersch, 2005; Connell, 2007; Jacques et al., 2008). As the real hydrologic system is usually composed of complex changing boundary conditions and heterogeneous and stratified formations, numerical models are more popular to handle complicated contaminant transport problems due to their flexibility to fit to complex boundary and initial conditions. Several numerical models have been developed, most of which are based on the Richards' equation to represent the water flow and the advection–dispersion equation (ADE) to represent the solute transport in the unsaturated–saturated system. A three-dimensional (3-D) model can provide the most appropriate simulation for many practical problems and is considered as the most rigorous approach (Pikul et al., 1974). The major drawback of the 3-D model is the large computational burden because of the intrinsic nonlinear nature of the 3-D Richards' equation (Pan and Wierenga, 1995; Miller et al., 1998; Berg, 1999), especially for the simulation in the vadose zone, where the size of grids should be in the order of cm to obtain the satisfactory accuracy (van Dam, 2000). Therefore, for the long term subsurface water flow and contaminant simulation in regional cases, the fully 3-D modeling is often very expensive. Moreover, the numerical stability problem when solving the nonlinear 3-D water flow equations is still a potential limitation, which would hamper the validity of the fully 3-D unsaturated–saturated model (Twarakavi et al., 2008).

Two groups of simplified models are developed to alleviate the computational burden. One is the quasi 3-D water flow and contaminant transport model, which reduces the 3-D equations to quasi 3-D formulations (Bredehoeft and Pinder, 1970; Neuman

* Corresponding author. Tel.: +86 2768775466.
E-mail address: jingwei.wu@whu.edu.cn (J. Wu).

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et al., 1982; Chorley and Frind, 1978; Huyakorn et al., 1986; Kuo et al., 2008; Lin et al., 2010; Paulus et al., 2013). The basic concept of these models is to layer the subsurface system into aquifers and aquitards. It is assumed that the 3-D flow components exist in the aquifer while only the vertical flow component exists in the aquitard. It is also similar to the so-called vertical/horizontal splitting (VHS) concept (Lardner and Cekirge, 1988; Tsai et al., 1998), which is widely used in the simplified modeling for the groundwater system by dividing the 3-D water flow equation into the depth averaged two-dimensional (2-D) equation and the vertical variation one-dimensional (1-D) equation.

The other type simplified model uses a simpler mathematical equation to represent the unsaturated water flow and solute transport. As field experiments show that the flux within the vadose zone mainly exists in the vertical direction, 1-D vertical water flow and solute transport equations may be sufficient to represent the flow and solute conditions (Romano et al., 1998; van Dam, 2000; Sherlock et al., 2002). Then by combining the 1-D unsaturated vertical flow and solute transport model with the 2-D or 3-D saturated water flow and solute transport model, the simplified unsaturated–saturated model can be established (Kool et al., 1994; Yakirevich et al., 1998; Rabbani and Warner, 1997; Li et al., 2007). Due to the computational technique and the specified research purpose, not only the unsaturated water flow and solute transport processes but also the saturated water flow and solute transport components are simplified in these models. The model established by Rabbani and Warner (1997) ignored the advection in the vertical direction in the aquifers. The model presented by Kool et al. (1994) was restricted to the steady-state groundwater flow. The model developed by Yakirevich et al. (1998) only simulated the 2-D groundwater flow and solute transport. Although the unsaturated flow mainly exists in the vertical direction for many regional-scale problems, the saturated water flow and contaminant transport is in a fully 3-D pattern (van Dam, 2000).

A more reasonable simplified unsaturated–saturated coupling model would require the integration of a 1-D unsaturated model with a 3-D saturated model. Several integrated unsaturated–saturated water flow models have been established based on this concept (Thoms et al., 2006; Niswonger et al., 2006; Seo et al., 2007; Twarakavi et al., 2008; Zhu et al., 2012b). These coupling models reduces simulation burden of regional-scale subsurface system significantly. The same concept is utilized to develop the unsaturated–saturated water flow and solute transport models (Christiansen et al., 2004; Herbst et al., 2005; Stenemo et al., 2005; Bergvall et al., 2011; Bergvall, 2011). In these models, a loose linking method is commonly adopted to couple the unsaturated and saturated solute transport equations. The calculated solute concentration from the bottom of the 1-D vadose zone model is used as the input to the 3-D groundwater model. The advantage of this coupling method is easy to program. However, the simulation accuracy will be influenced significantly by the linkage depth since the two models are run separately and there is no feedback between them (Stenemo et al., 2005). Another problem concerned the 1-D unsaturated model coupling with MODFLOW (Harbaugh et al., 2000) and MT3D (Zheng and Wang, 1999) is the arbitrary mesh generation for irregular domain boundaries (Bergvall et al., 2011).

The objective of this study is to establish a fully integrated numerical model to predict unsaturated–saturated solute transport at the regional scale. It is an extension of our former work, which proposed a coupling model for the regional-scale unsaturated–saturated water flow simulation (Zhu et al., 2012b). The 1-D ADE and the 3-D ADE are adopted to describe the solute migration through the unsaturated zone and the saturated zone. A novel integrated method is implemented to assemble the two equations into one unified matrix, which is solved simultaneously to yield the satisfactory convergence performance. Four cases are carried out to test the validity of the model. The limitations and computational efficiency of the model are discussed as well.

2. Model development

2.1. Assumptions and methodology

The solute transport model is developed based on the coupling water flow model in our former work (Zhu et al., 2012b). In the coupling water flow model, the simulation domain is partitioned into a number of sub-areas in the horizontal direction mainly according to the spatially distributed inputs (e.g. soil materials, atmosphere boundary conditions, and land use types). A 1-D soil column is assigned to each sub-area to characterize the average unsaturated water flow in that sub-area. The 1-D unsaturated and 3-D saturated modules are then integrated by implicitly expressing the vertical flow flux between the unsaturated and saturated zones. In this study, an integrated solute transport model is further established to couple with the water flow model. Three major assumptions are made in the current work, (1) the solute transport through the unsaturated zone mainly exists in the vertical direction; (2) the solute transport in the saturated zone occurs in three dimensions but there is only the vertical solute mass exchange between the unsaturated and saturated zones; and (3) the possible advection and dispersion along the horizontal direction are ignored in the unsaturated zone.

Under these assumptions, the solute transport in the unsaturated zone is represented by the 1-D ADE, and the fully 3-D ADE for the saturated zone. The 1-D ADE is discretized by the finite element method. The discretization of the saturated solute transport equation is implemented by splitting the 3-D ADE into the horizontal and vertical equations, which is similar with the VHS concept. Mass balance analyses for the adjacent nodes in the unsaturated zone and at the water table are elaborated in Section 2.4 to help to formulate the integrated solute migration matrix. The implementation technique of coupling the unsaturated solute transport module with the saturated module is presented with a hypothetical example.

2.2. Solute transport equations

The contaminant transport is described by the ADE with the linear adsorption/desorption, zero-order and first-order reactions, and source/sink terms,

$$\frac{\partial \theta R c}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial c}{\partial x_j}\right) - \frac{\partial q_i c}{\partial x_i} - F_1 c + G, \tag{1}$$

where R is the retardation factor defined as [-],

$$R = 1 + \frac{\rho k}{\theta}, \tag{2}$$

and F_1 is the first-order term [T^{-1}], and G is the zero-order term [$ML^{-3}\,T^{-1}$]. F_1 and G can be defined as,

$$F_1 = \mu_w\theta + \mu_s\rho k, \tag{3}$$
$$G = \gamma_w\theta + \gamma_s\rho - Sc_s. \tag{4}$$

In Eqs. (1)–(4), θ is the volumetric water content [-]; c is the solute concentration [ML^{-3}]; t is the time (T); x_i, x_j (i, j = 1, 2, 3) are the spatial coordinates [L]; q_i (i = 1, 2, 3) are the water fluxes in the three directions [LT^{-1}]; ρ is the bulk density [ML^{-3}]; k is the empirical constant when using a linear equation to represent the equilibrium interactions between the solution concentration and the adsorbed solute concentration in the soil [$L^3\,M^{-1}$]; μ_w is the first-order rate constant for solutes in the liquid phase [T^{-1}]; μ_s is the