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Switching the Richards' equation for modeling soil water movement under unfavorable conditions

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ABSTRACT

Simulation of variably saturated soil water flow requires the use of pressure head, or soil moisture, or a switching between the two, as the primary variable for solving Richards' equation. Under unfavorable conditions, such as heterogeneity, rapidly changing atmospheric boundary, or sudden infiltration into dry soils, the traditional non-switching method suffers from numerical difficulties. Solving this problem with a primary variable switching method is less preferred due to the mathematical complexity. While the Picard method is more popular for solving the non-switching models due to its simplicity and stability, two different forms of Richards' equation are combined into one numerical scheme for switching under specific hydraulic conditions. The method is successfully implemented in a one-dimensional model solved by a Picard iteration scheme. A threshold saturation based on the soil moisture retention relation is used for switching between either form of the Richards' equation. The method developed here is applicable for simulating variably saturated subsurface flow in heterogeneous soils. Compared with traditional methods, the proposed model conserves mass well and is numerically more stable and efficient.

1. Introduction

The Richards' equation (RE, (Richards, 1931)) is considered the only basis for accurate and physically-based solutions for modeling the sub-surface flow (Farthing and Ogden, 2017). However, the significant non-linearity of moisture retention curves has led to major efforts to improve the generality and efficiency of algorithms for solving RE, either analytically (White and Broadbridge, 1988), or numerically (Forsyth et al., 1995; Ross, 2003; Zha et al., 2017). In spite of the limitations of analytical methods (Crevoisier et al., 2009), numerical schemes for solving different forms of RE still suffer from problems of robustness and accuracy (Krabbenhøft, 2007; Ross, 2003; Zha et al., 2017, 2013a,b), particularly for infiltration into dry soils with a sharp wetting front, rapidly changing atmospheric upper boundary conditions, as well as heterogeneous soils.

The primitive form of the one dimensional RE, also called the mixed-form RE, is derived from the mass balance equation

$$\partial\theta/\partial t = -\partial q/\partial z \tag{1}$$

and Darcy's law

$$q = -K\frac{\partial h}{\partial z} + K \tag{2}$$

where θ [L^3L^{-3}] is the volumetric soil moisture content, t [T] is the time, z [L] is the spatial location (positive downward), and q [LT^{-1}] is the vertical Darcian flux, h [L] is the pressure head, K [LT^{-1}] is the hydraulic conductivity. Generally, Eqs. (1) and (2) contribute to the mixed form RE, in which the pressure head (h) serves as the driving force variable, and soil moisture (θ) as the accumulation variable (Krabbenhøft, 2007). To be solved numerically, either θ or h is preferentially taken as the primary variable. When the Darcian flux (Eq. (2)) is substituted with $q = -D\cdot\partial\theta/\partial z + K$, where D [L^2T^{-1}] is the hydraulic diffusivity, the conventional *θ-form* RE results

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial\theta}{\partial z}\right) - \frac{\partial K}{\partial z} \tag{3}$$

Alternatively, by replacing the storage term in Eq. (1) with $\partial\theta/\partial t = C\cdot\partial h/\partial t$, where C [L^{-1}] is the soil capacity ($C = \partial\theta/\partial h$), the *h-form* RE follows:

$$C\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z}\right) - \frac{\partial K}{\partial z} \tag{4}$$

The *θ-form* RE is inherently mass conservative and less non-linear (Warrick, 1991) in the inter-nodal averaged hydraulic diffusivity D, especially for dry soil conditions, thus reducing the numerical difficulties. Furthermore, in terms of experimental measurement, available

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devices for monitoring soil moisture are directly applicable for model calibration and parameter estimation (Robinson et al., 2008). However, models based on *θ-form* RE cannot properly account for the inter-nodal flux terms when there are saturated nodes or in heterogeneous soils (Crevoisier et al., 2009; Kirkland et al., 1992; Zha et al., 2013b). Although improved approximation of flows in heterogeneous soils have been achieved (Matthews et al., 2004; Schiesser, 1991; Zha et al., 2013b), the *θ-form* methods cannot deal with saturated soils or mixed unsaturated/saturated situations.

In contrast, the *h-form* methods are more general for variably saturated flow simulation, especially in heterogeneous soils. However, they usually lead to serious mass balance errors (Celia et al., 1990). With Celia's mass balance scheme, some popular codes/software packages based on the *h-form* RE have been developed (Šimůnek et al., 2009; van Dam et al., 2008). Nevertheless, such mass balance errors are largely determined by the iteration closure criteria. Furthermore, in the *h-form* model, the nonlinearity of both the soil water capacity $C(h)$ and the hydraulic conductivity $K(h)$, as well as the non-monotonicity of $C(h)$, contribute jointly to instabilities when simulating infiltration into dry soil (Zha et al., 2017).

To reduce the nonlinearity of the head in the unsaturated zone while preserving model generality, a so-called primary variable switching technique has been proposed by taking either h or θ as the primary variable, depending on the saturation of the numerical nodes (Diersch and Perrochet, 1999; Forsyth et al., 1995). Under a Newton's iteration framework, the primary variable switching technique takes the derivative of the discretized equation set with respect to h for saturated nodes, or with respect to θ for unsaturated nodes (Brunner and Simmons, 2012; Diersch and Perrochet, 1999; Forsyth et al., 1995; Krabbenhøft, 2007; Wu and Forsyth, 2001). The resultant Jacobian matrix is used to solve the equation set with increments of primary variables (Δh or $\Delta\theta$) as unknowns. After solving the increments, the primary variables and their corresponding secondary variables are updated, and the simulation proceeds. However, such an algorithm inevitably causes non-smooth transitions between alternative primary variables, which potentially produce unrealistic solutions (Krabbenhøft, 2007; Zha et al., 2017). Although improvements were made to minimize such deficiencies (Hassane Maina and Ackerer, 2017; Kees and Miller, 2002; Krabbenhøft, 2007), the schemes tend to be problem specific. Additionally, the proposed switching method has been restricted to Newton's iteration methods. Although more robust and with higher-order convergence than the Picard method (Paniconi and Putti, 1994), Newton's method increases algebraic complexity and computational costs for assembling the derivative terms in the Jacobian matrix (Krabbenhøft, 2007; Paniconi and Putti, 1994). Several popular numerical codes of RE, such as HYDRUS (Šimůnek et al., 2008) and SWAP (van Dam et al., 2008), are designed for Picard method.

Based on the above, a generalized method that reduces the nonlinearity of the head in the unsaturated zone while keeping model generality is developed in this paper. We directly start from the *h-form* RE (Eq. (4)) for saturated regions while the *θ-form* RE (Eq. (3)) for unsaturated regions. The numerical discretization of a computational element bounded by two nodes is handled by combining the *h-* and *θ-form* REs at the equation level. The resulting numerical model uses head and moisture as unknown variables for saturated and unsaturated nodes respectively. From an implementation perspective, the proposed method is more general since it can be used in both Picard and Newton iteration schemes. Moreover, to alleviate the non-smooth transition between alternative primary variables (Krabbenhøft, 2007), a threshold effective saturation of Se^{crit} is employed to regulate the primary variable switching within the Picard iteration scheme.

The paper is arranged as follows: the generalized numerical scheme for switching between the two governing REs is given in Section 2; examples of its use in numerical experiments is presented in Section 3, where a remarkable increase in model robustness is achieved using the proposed method. Results and discussion are in Section 4 and conclusions are reached in Section 5.

2. Numerical formation

2.1. Numerical solution of Richards' equation

The generalized RE in two different forms is derived by combining Eqs. (3) and (4) into

$$\beta\frac{\partial\Phi}{\partial t}=\frac{\partial\Phi}{\partial z}\left(\hat{K}\frac{\partial\Phi}{\partial z}\right)-\frac{\partial K}{\partial z} \tag{5}$$

where Φ is the primary variable for two different forms of RE. The effective saturation at each node, Se, is used to determine the form of RE at node i. When $Se > Se^{crit}$, an *h-form* RE is taken as the governing equation, thus we get $\Phi = h$, $\hat{K} = K$, and $\beta = C$; or else when $Se < Se^{crit}$, a *θ-form* RE is used, then $\Phi = \theta$, $\hat{K} = D = K/C$, and $\beta = 1$. The switching threshold Se^{crit} is of great dependence on the soil parameters and hydraulic conditions near the dry-wetting front. In our work, a range of empirical Se^{crit} from 0.4 to 0.99 are suggested.

At spatial location z and time t, the Dirichlet and Neumann boundary conditions are described by

$$\Phi(z,t)=\Phi_0(z,t) \text{ and } \hat{K}(z,t)\frac{\partial\Phi(z,t)}{\partial z}-K(z,t)=q_0(z,t) \tag{6}$$

where Φ_0 and q_0 [LT^{-1}] are respectively the known value of the primary variable and inter-nodal flux.

With a vertex-centered finite-difference grid and a backward-Euler finite-difference stepping scheme, the spatial and temporal parts in Eq. (5) are integrated into the matrix equations as follows

$$\mathbf{f}(\mathbf{\Phi}^{j+1})=\mathbf{A}(\mathbf{\Phi}^{j+1})\mathbf{\Phi}^{j+1}+\mathbf{B}(\mathbf{\Phi}^{j+1})\frac{\mathbf{\Phi}^{j+1}-\mathbf{\Phi}^{j}}{\Delta t^{j+1}}-\mathbf{F}(\mathbf{\Phi}^{j+1})=0 \tag{7}$$

where the superscript j denotes the time level, Δt^{j+1} is the current time step, $\Delta t^{j+1}=t^{j+1}-t^{j}$; $\mathbf{A}$ is a symmetrical tri-diagonal matrix assembled by $\mathbf{A}=\sum_e \mathbf{A_e}$, where $\mathbf{A_e}$ is the element stiffness matrix, at element $i-1/2$,

$$\mathbf{A_e}=\begin{bmatrix}\frac{\hat{K}_{i-1/2}^{j+1}}{\Delta z_{i-1/2}} & -\frac{\hat{K}_{i-1/2}^{j+1}}{\Delta z_{i-1/2}}\\ -\frac{\hat{K}_{i-1/2}^{j+1}}{\Delta z_{i-1/2}} & \frac{\hat{K}_{i-1/2}^{j+1}}{\Delta z_{i-1/2}}\end{bmatrix} \tag{8}$$

$\mathbf{B}$ is a diagonal matrix for storage terms assembled by $\mathbf{B}=\sum_i B_i$, at node i,

$$B_i=\Delta z_i\beta_i=\begin{cases}\Delta z_i C_i^{j+1}, & Se_i > Se^{crit}\\ \Delta z_i, & Se_i < Se^{crit}\end{cases} \tag{9}$$

and $\mathbf{F}$ is a vector for gravity and sink/source terms assembled by $\mathbf{F}=\sum_e \mathbf{F_e}$. The component from element $i-1/2$ is represented by

$$\mathbf{F_e}=\begin{Bmatrix}-K_{i-1/2}^{j+1}\\ K_{i-1/2}^{j+1}\end{Bmatrix} \tag{10}$$

where $\Delta z_i=(z_{i+1}-z_{i-1})/2$ is the size of control volume of the vertex-centered node i; $\Delta z_{i-1/2}=z_i-z_{i-1}$ is the size of the finite element bounded by nodes $i-1$ and i; $\hat{K}_{i-1/2}=(\hat{K}_i+\hat{K}_{i-1})/2$ is the inter-nodal average hydraulic parameter, when $Se_i > Se^{crit}$, $\hat{K}_i=K_i$, while when $Se_i < Se^{crit}$, $\hat{K}_i=D_i$; Specifically, $K_{i-1/2}$ in Eq. (10) is the inter-nodal average hydraulic conductivity for element $i-1/2$, $K_{i-1/2}=(K_i+K_{i-1})/2$. When using an *h-form* RE, the Celia format (Celia et al., 1990) for temporal discretization is employed to conserve mass.

Solving Eq. (7) with a quadratic-convergence iteration scheme (Newton's scheme) leads to

$$\mathbf{f}'(\mathbf{\Phi}^{j+1,k})(\mathbf{\Phi}^{j+1,k+1}-\mathbf{\Phi}^{j+1,k})+\mathbf{f}(\mathbf{\Phi}^{j+1,k})=0 \tag{11}$$

where k is the iteration level, and $\mathbf{f}'(\mathbf{\Phi}^{j+1,k})$ is the Jacobian matrix, its