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A mass-conservative switching algorithm for modeling fluid flow in variably saturated porous media

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ABSTRACT

Numerical solutions of flow equation in fluid content-based form or in fluid pressure head-based form are often tradeoffs between speed, accuracy, and convenience. The fluid-content based form can be solved quite rapidly with low CPU time and perfect mass balance. However, it cannot be used in saturated regions (as diffusivity function becomes infinite) and strictly becomes invalid in composite, layered, and *real* heterogeneous porous materials, due to singularity and discontinuity in fluid content profile. This formulation also gives misleading impression that gradient in fluid content causes the flow of fluid in porous materials, where in reality gravity and fluid pressure potential gradient produce the motion. The pressure head-based form, on the other hand, is more flexible but due to its highly nonlinear nature is much more time-consuming and produces poor global mass balance for dry initial conditions. Very fine spatial and temporal discretizations are needed to maintain mass balance property for these scenarios. The mixed form of the flow equation partially solves these issues as it maintains acceptable mass balance and is applicable to layered, heterogeneous, and composite fractured foundations. However, it is only applicable in unsaturated zones. In this study, a switching algorithm was proposed and implemented in which the mass conservative mixed form and the pressure head-based form were, respectively, used in the unsaturated and saturated zones of an initial-boundary value flow problem involving a variably saturated porous medium. The algorithm showed excellent agreement with a reference solution, obtained on a very fine spatiotemporal mesh. The simulator was then calibrated with several real-world large-scale experimental datasets. In all cases, the proposed algorithm exhibited close agreements with the experimental time–space series. The algorithm poses excellent mass balance property and can easily be used in both saturated and unsaturated regions without special treatment of fluid content discontinuities in heterogeneous and layered porous media. The proposed algorithm can also be extended to simulate multiphase and multidimensional flow problems.
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1. Introduction

Fluid flow in variably saturated porous media plays an important role in many branches of sciences and engineering including petroleum reservoir [3], multi-phase flow [2,14], water resources [46,50,51], and bioenvironmental processes [53,54]. Experimentation and process-based mathematical modeling are two orthodox approaches which have been extensively used to analyze fluid flow in different systems with varying degree of complexity. While experimentation may better represent the micro- and macro-environment of the systems; they are time-consuming, tedious, expensive, and often impose unrealistic and simplified initial and boundary conditions on transport domain and processes in, especially, open

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systems [55]. An efficient alternative is developing state-of-the-art process-based mathematical models with enhanced prediction capabilities. The success of mathematical models in describing, understanding, and predicting the dynamics of the systems depends largely on proper representation of relevant physical, chemical, and biological processes, parameter identification, and uncertainty in model parameters [52].

Mathematical modeling of fluid flow in variably saturated porous media usually results in systems of highly nonlinear partial differential equations which are not solvable analytically unless unrealistic and oversimplifying assumptions are made regarding the attributes, dynamics, and properties of the physical systems. While analytical solutions are useful for a number of applications such as verification of numerical simulators [48] and approximate determination of fluid properties, their over-simplified nature reduces their predictive capabilities. Therefore, numerical solutions are usually the only viable procedures to model flow and transport phenomena in partially saturated porous media. The standard numerical schemes are finite volume, finite element, and finite difference methods which are usually coupled with an Euler time discretizations scheme. Except for the fully explicit forward method, any other Euler time-marching algorithm generates nonlinear algebraic equations which should be solved using iterative procedures such as Newton and Picard algorithms.

In modeling flow in variably saturated porous media, most attention has been paid to overcoming the nonlinearity of flow and mass transport problems and reducing numerical dispersion and artificial oscillations of the numerical simulators. In comparison, little efforts have been directed to elimination or reduction of mass balance error. Mass balance is defined as the ratio of the total masses of fluid added to the domain to the total net flux into the domain [5]. An accurate numerical simulator should conserve mass over entire spatiotemporal domain. A standard approach to reduce mass balance error in a highly nonlinear equation or a set of coupled nonlinear equations is using small time steps and iterative procedures, which in turn makes the solution very time consuming. As Huang et al. [19] noticed and will be demonstrated in this study; for some problems, depending on the nature and severity of the nonlinearity, global mass balance errors may not be totally eliminated even when very small time steps are used.

The goal of this study is to critically evaluate the global mass balance error of the numerical simulators of flow equation in porous media, develop and evaluate a mass-conservative switching algorithm, and conduct large-scale experiment in a real-world open system to collect required data sets to test the efficacy, accuracy, and mass balance property of the numerical simulator in solving an initial-boundary value problem which simulates flow through partially saturated porous media. The algorithm uses the mixed form Richards equation in unsaturated zone and switches to pressure head-based form in and near the saturated region. Realistic initial and Dirichlet as well as Neumann boundary conditions are imposed in the numerical simulator and the corresponding physical models to gather experimental data. To reduce CPU time and maintain small truncation error, an adaptive time-stepping strategy is developed and implemented. The nonlinear matrix equations are solved using the modified Picard iteration scheme. The performance of the algorithm is shown to be superior to the conventional pressure head-based form and can easily be used in layered porous media without special treatment of fluid content discontinuities.

The plan of the paper is as follow: in Section 2, the partial differential equations governing fluid flow in partially saturated porous media and the corresponding numerical simulators are presented. Bothe finite element and finite difference approximations are considered. The modified Picard algorithm is presented in this section followed by the implementation of the adaptive time-stepping strategy. The proposed switching algorithm is presented in Section 3. Formulation of the global mass balance error is given in Section 4 followed by the model validation in Section 5. Implementation, model calibration, numerical test problems, and analysis of the results are presented in Section 6 followed by concluding remarks in Section 7.

2. Governing equations and discretizations

The laws of hydrodynamics govern the flow of fluids in variably saturated porous media, where gravity and fluid pressure gradient produce the motion [43,45,46,50]:

$$\frac{\partial \theta}{\partial t} - \nabla \cdot K(h)\nabla h + \frac{\partial K}{\partial z} = 0 \tag{1}$$

where θ is fluid content of porous medium ($L^3\,L^{-3}$), h is fluid pressure head (L), $K(h)$ is capillary conductivity function ($L\,T^{-1}$), z is vertical coordinate (L), assumed positive downward, and t is time (T). Eq. (1) is known as the *mixed-form Richards* equation [5]. Using the chain rule of differentiation, the fluid content based (θ-based):

$$\frac{\partial \theta}{\partial t} - \nabla \cdot D(\theta)\nabla \theta + \frac{\partial K}{\partial z} = 0 \tag{2}$$

and the fluid pressure head based (h-based):

$$C(h)\frac{\partial h}{\partial t} - \nabla \cdot K(h)\nabla h + \frac{\partial K}{\partial z} = 0 \tag{3}$$

forms of (1) have been developed [5,46]; where $C(h) = d\theta/dh$ is specific fluid capacity (L^{-1}) function (the rate of change of the fluid content of the medium with respect to fluid pressure head) and $D(\theta) = K(\theta)dh/d\theta = K(\theta)/C(\theta)$ is fluid diffusivity function ($L^2\,T^{-1}$). Notice that fluid pressure, unsaturated hydraulic conductivity, and specific fluid capacity (capacitance) are analogous, respectively, to temperature, thermal conductivity, and thermal capacity in heat transfer. A thorough discussion will be given, below Eq. (10), on the myth and misconceptions regarding the use of (2) in porous media community.

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