Advanced Numerical Techniques in Modeling Unsaturated Flow

Abstract

Primary variable switching can overcome the most of the numerical difficulties arising in the simulation of variably saturated flows. The technique is incorporated in both an adaptive error-controlled predictor-corrector one-step Newton (PCOSN) iteration strategy and a target-based full Newton (TBFN) iteration scheme for finite elements in two and three dimensions. Examples are presented to show the power of the proposed new schemes.

Kurzfassung


1 Introduction

Flow and transport processes in the unsaturated (vadose) zone play a major role in a wide variety of engineering problems ranging from groundwater recharge, dam seepage, capillary barriers, drainage and flooding (Diersch, 1998a), via contamination by surface spills of pollutants or salinity displacements in soils, up to heat transport in soils and drying processes in porous media. Several alternatives exist to solve numerically the governing balance equations with their nonlinear constitutive relationships. The Darcy equation of fluid motion and the fluid mass conservation equation form the physical basis [Bear and Bachmat, 1991]. In the context of unsaturated flow the basic formulation possesses both the fluid pressure head $\psi$ and the saturation $s$ as unknown variables to be determined. For these two unknowns only one balance equation, the basic Richards equation, is available. To close the mathematical model one constitutive relationship in form of the capillary pressure head-saturation function is additionally needed to convert the one variable to the other (and vice versa).
Consequently, the modeler has to decide between primary and secondary variables. Dependent on such a choice, different modeling approaches result which are mathematically equivalent in the continuous formulation, but their discrete analogs are quite different.

As the result, three forms of the unsaturated flow equation can be derived: (1) the pressure-based (\(\psi\)-)form, where the primary variable is the pressure head (or the hydraulic head), (2) the saturation-based (\(s\)-)form, where the saturation (or the moisture content \(\theta\)) is chosen as the primary variable, and (3) the mixed (\(\psi - s\)-)form, where both variables are applied, however, in solving the discrete equation system the pressure head is actually used as the primary variable.

Each of the different forms has its advantages and drawbacks: The \(\psi\)-based form can be used for both saturated and unsaturated soils. The pressure head variable is unique and continuous. But, the \(\psi\)-based form can produce significant global mass balance errors unless very small time steps are used. On the other hand, the mixed (\(\psi - s\)-)form provide much better properties with respect to accurate mass conservative solutions. Usually, modified Picard and the Newton methods are used for solving the nonlinear Richards equation in the mixed form with the pressure head as the chosen primary variable. Alternatively, numerical schemes which are based on the \(s\)-form of the Richards equation are restricted to unsaturated flow conditions because the saturation variable is not unique for saturated regions, where the soil-water diffusivity goes to infinity and a pressure-saturation relationship does not more exist. But it is interesting to note that a saturation-based algorithm can result in a significantly improved performance compared to pressure-based methods, especially when very dry heterogeneous soils are modelled.

Recently, Forsyth et al. [1995] introduced a powerful new idea in the context of saturated-unsaturated flow simulations. It is termed as the primary variable switching technique which is originated in multiphase modeling to handle effectively the appearance and disappearance of phases. A full Newton method is used where the different primary variables in form of saturation and pressure are switched in different regions in dependence on the current saturation condition at each node of a mesh. This technique has found to produce rapid convergence in both the unsaturated and saturated zones compared with pressure-based formulations. In this light, primary variable switching appears as a promising technique to speed-up the overall solution process and to tackle difficult-to-solve problems for unsaturated-saturated flows. In the present paper modifications and improvements of Forsyth et al.'s scheme are done with respect to an embedding into a powerful predictor-corrector approach with first and second order accuracy, the use of a one-step full Newton approach with only one control parameter to manage the entire solution process in an adaptive time marching scheme, and in a rigorous analytical derivation of the Jacobian of the Newton method. In
contrast to the predictor-corrector solution control an aggressive target-based
time marching scheme is studied which will provide an effective but error-prone
strategy.

2 Basic Equations
The mass conservation equation of a fluid in a variably saturated media is given
by [Bear and Bachmat, 1991]

\[ S_0 \cdot s(\psi) \frac{\partial \psi}{\partial t} + \varepsilon \frac{\partial s(\psi)}{\partial t} + \nabla \cdot q = Q \] (1)

The fluid motion is described by the Darcy equation written in the form

\[ q = -K_r(s)K [\nabla \psi + (1 + \chi) e] \] (2)

In (1) and (2),

- \( \psi \): pressure head, \((\psi > 0 \text{ saturated medium}, \psi \leq 0 \text{ unsaturated medium})\);
- \( s(\psi) \): saturation, \((0 < s \leq 1, s = 1 \text{ if medium is saturated})\);
- \( q \): Darcy flux vector;
- \( t \): time;
- \( S_0 \): specific storage due to fluid and medium compressibility;
- \( \varepsilon \): porosity;
- \( K_r(s) \): relative hydraulic conductivity \((0 < K_r \leq 1, K_r = 1 \text{ if saturated})\);
- \( K \): tensor of hydraulic conductivity for the saturated medium;
- \( \chi \): buoyancy coefficient including fluid density effects;
- \( e \): gravitational unit vector;
- \( Q \): specific mass supply;

Constitutive relationships are additionally required for the saturation \( s \) as a
function of the pressure (capillary) head \( \psi \), with its inverse, the pressure head \( \psi \) as a function of the saturation \( s \), and for the relative hydraulic conductivity \( K_r \) as a function of the pressure head \( \psi \) or the saturation \( s \). Empirical relationships are given by the van Genuchten-Mualem, the Brooks-Corey or the Haverkamp parametric models [Bear and Bachmat, 1991].

3 Finite Element Formulation
Using the Galerkin-based finite element method in two and three dimensions the
following global matrix system of \( M \) equations results
\[
O(s) \cdot \dot{\Psi} + B \cdot \dot{s} + K(s) \cdot \Psi - F(s) = 0
\]  
(3)

The superposed dot means differentiation with respect to time \( t \). Nonlinearities are shown in parenthesis. Notice, all matrices connected with time derivatives are lumped which is virtually mandatory for unsaturated problems to guarantee smooth and nonoscillatory solutions. The system of equations (3) is highly nonlinear due to the nonlinear dependence in the constitutive relationships for the saturation and the relative conductivity.

From stability reasons only implicit (A-stable) time discretizations are appropriate for the present class of problems. Otherwise, two-step techniques have to be preferred for multidimensional problems due to practical implications. Denoting the time plane by the superscript \( n \) and inserting difference approximations for the time derivatives the following general matrix system finally results

\[
R^{n+1}(\Psi, s) =
\left( \frac{\sigma O(s^{n+1})}{\Delta t_n} + K(s^{n+1}) \right) \cdot \Psi^{n+1} + \frac{\sigma B}{\Delta t_n} \cdot s^{n+1} - O(s^{n+1}) \cdot \left( \frac{\sigma}{\Delta t_n} \Psi^n + (\sigma - 1) \dot{\Psi}^n \right) - B \cdot \left( \frac{\sigma}{\Delta t_n} s^n + (\sigma - 1) s^n \right) - F(s^{n+1})
\]

\[= 0\quad (4)\]

where the weighting factor \( \sigma \in (1, 2) \) differs between first order and second order temporal discretization schemes.

### 4 Primary Variable Switching Methodology

To solve the basic matrix system (4) one has to decide which variable should be primary, either \( \psi \) or \( s \). Commonly, the selection of the primary variable is done in a static manner. As the result the modeling strategy becomes fixed as \( \psi - s \) or \( \psi - s \)-forms as discussed above regarding their limitations and drawbacks. In contrast, the idea of primary variable switching is general, however, quite simple: The selection of the primary variable is to do dynamically in dependence on the current flow characteristics.

Let \( X_I \) be the primary variable associated with node \( I \). \( X_I \) can be either \( \psi_I \) or \( s_I \). Accordingly, we can consider \( X \) as a vector containing the different primary variables in the solution space:

\[
X \in (\Psi, s) \quad (5)
\]
The matrix system (4) can be written in the condensed form

$$ R^{n+1}_I (X) = 0 $$

(6)

for seeking the solution $X_I$ of a system of $M$ equations ($I = 1, \ldots, M$).

The solution of the nonlinear equations (6) for the $M$-vector of primary variables $X$ is performed by the Newton method, viz.,

$$ J^X \left( \Psi^{n+1}_{\tau}, s^{n+1}_{\tau} \right) \Delta X^{n+1}_{\tau} = -R^{n+1}_{\tau} (\Psi, s) $$

(7a)

with the increment

$$ \Delta X^{n+1}_{\tau} = X^{n+1}_{\tau+1} - X^{n+1}_{\tau} $$

(7b)

and the Jacobian $J^X$ written in indicial notation

$$ J^X_{IJ} \left( \Psi^{n+1}_{\tau}, s^{n+1}_{\tau} \right) = \frac{\partial R^{n+1}_I (\Psi^{n+1}_{\tau}, s^{n+1}_{\tau})}{\partial X^{n+1}_{\tau J}} $$

(7c)

where $\tau$ denotes the iteration number.

The primary variable at any given node $I$ is switched for every Newton iteration $\tau$ by using the following method:

**IF** ($s^{n+1}_{\tau I} \geq tol_f$) **THEN**

Use $\psi^{n+1}_{\tau I}$ as primary variable at node $I$ and solve the Newton statement (7a) as

$$ J^\Psi_{IJ} \left( \psi^{n+1}_{\tau}, s^{n+1}_{\tau} \right) \Delta \psi^{n+1}_{\tau J} = -R^{n+1}_{\tau I} (\Psi, s) $$

(8)

**ELSE IF** ($s^{n+1}_{\tau I} < tol_b$) **THEN**

Use $s^{n+1}_{\tau I}$ as primary variable at node $I$ and solve the Newton statement (7a) as
Do not change primary variable for the node $I$ and solve (8) or (9) according to the hitherto selected primary variable ($\psi_{\tau I}^{n+1}$ or $s_{\tau I}^{n+1}$).

ELSE

ENDIF

5 Solution Control

Generally, the control of the solution of the resulting highly nonlinear matrix systems (8) and (9) is a complicated task. The choice of the time step size $\Delta t_n$ and the iteration control of the Newton scheme influence significantly the success and the efficiency of the simulation. On the other hand, it is to be required that the overall solution process should be performed at a minimum of user-specified control parameters. It becomes clear only a fully automatic and adaptive time selection strategy can be useful for the present class of problems. In this work both a predictor-corrector one-step Newton (PCOSN) time integrator and a target-based full Newton (TBFN) scheme with aggressive time step size selection are applied. A detailed description of these techniques is given by Diersch and Perrochet [1998]. It should be emphasized the PCOSN technique controls the overall temporal discretization error via a truncation error criterion. This error-controlled solution strategy is in contrast to the TBFN. In the TBFN technique the step size is controlled so that the Newton corrections hit, or are less than, target change parameters. It makes usage of the fact that the used formulation is mass-conservative for an arbitrary implicit step size. Actually, this aggressive time stepping control can be very effective in finding steady-state solutions, if ever exist, but in transient situations it appears as an error-prone strategy in a potential lacking of temporal accuracy. This is regardless of the good mass-conservative properties possessing the scheme.

6 Examples

6.1 Infiltration in a Large Caisson

The infiltration process in a large caisson of a heterogeneous material at dry initial conditions has been thoroughly studied by Forsyth et al. [1995]. We take up this problem to show the power of the variable switching technique and to indicate the differences in the solutions caused by the time stepping and iteration control alternatives. Figure 1 presents the schematic view of the two-dimensional cross-sectional problem. Two different initial pressure head $\psi^0$ conditions have been studied.
The TBFN scheme became about four times faster than the PCOSN scheme as listed in Table 1. The extra costs for the PCOSN scheme are reflected in an increased temporal accuracy so as required by the error control. The results at simulation time of 30 days can be seen in Figure 2 for $\psi^0 = -7.34$ m in comparison with Forsyth et al.'s findings. Surprisingly, the PCOSN results are rather depart from the TBFN. The saturation front is significantly diffused in the 'low-cost' TBFN simulation while the PCOSN provides a much steeper saturation profile. The example distinctly illustrates how far a seemingly accurate, convergent and efficient solution can be from a more accurate prediction. It is apparent the present problem is sensitive with respect to discretization errors. The influence of the spatial discretization is evidenced in Figure 3 for the case of $\psi^0 = -100$ m. The results of structured coarse meshes are compared with a sufficiently dense unstructured mesh consisting of 56,960 triangular elements (28,917 nodes). For more details see Diersch and Perrochet [1998].

![Fig. 1 Infiltration problem (modified from Forsyth et al. [1995]).](image)

<table>
<thead>
<tr>
<th></th>
<th>$\psi^0 = -7.34$ m</th>
<th>$\psi^0 = -100$ m</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PCOSN</strong></td>
<td>Time steps</td>
<td>Total Newton steps</td>
</tr>
<tr>
<td></td>
<td>199</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>279</td>
<td>279</td>
</tr>
<tr>
<td><strong>TBFN</strong></td>
<td>15</td>
<td>51</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>69</td>
</tr>
</tbody>
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Table 1. Solution effort for the infiltration problem
Fig. 2 Computed saturation contours at $t = 30$ d, initial pressure head $\psi^0 = -7.34$ m: a) present solutions by PCOSN and TBFN; b) Forsyth et al.'s [1995] results.

Fig. 3 Influence of spatial discretization, computed saturation contours at $t = 30$ d, initial pressure head $\psi^0 = -100$ m: dense mesh consists of 56,960 triangles and 28,917 nodes, PCOSN strategy.

6.2 Capillary Barrier Modeling

A capillary barrier arises in unsaturated flow conditions at the contact of a fine layer of soil overlying a coarse layer of soil. If such a contact is tilted, infiltrating moisture in the fine layer will be diverted and flow down the contact as capillary diversion. To simulate such a capillary barrier numerical schemes have to tackle large parameter contrasts, highly exaggerated and rotated geometric relationships as well as very dry initial conditions.

We study a capillary barrier problem which has been recently considered by
Forsyth and Kropinski [1997]. The problem is described in Figure 4. As indicated the initial conditions are very dry.

As shown in Figure 5 the computed saturation streamline patterns reveals that the diversion is obviously more than 10 m. Actually, considering the velocity distribution along a section through the tuff the leakage increases from zero at about 10 m to the infiltration rate at about 25 m over a transition zone as depicted in Figure 6. The evaluation of an analytical formula in using the van Genuchten parameter of the sand and gravel zones gives an estimation of the diversion length of about 17.9 m, which agrees quite well with the present numerical simulations as also evidenced in Figure 6.

<table>
<thead>
<tr>
<th>Zone</th>
<th>( \psi^0 ) [kPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loam</td>
<td>(-10^6)</td>
</tr>
<tr>
<td>Sand</td>
<td>(-10^6)</td>
</tr>
<tr>
<td>Gravel</td>
<td>(-30)</td>
</tr>
<tr>
<td>Crushed tuff</td>
<td>(-6 \cdot 10^{10})</td>
</tr>
</tbody>
</table>

Fig. 4 Capillary barrier model domain (modified from Forsyth and Kropinski [1997]).

Fig. 5 Simulated saturation and streamline patterns at \( t = 1100 \) years by using TBFN.
7 Closure

The primary variable switching technique has proved to be a powerful and cost-effective solution strategy for unsaturated flow problems. Compared to conventional approaches based on the $\psi$-form and the mixed $\psi - s$-form of the Richards equation the primary variable switching technique can reduce the solution effort by orders. The described schemes have been implemented in the FEFLOW package [Diersch, 1998b] for two-dimensional and three-dimensional problems.

8 References


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