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A numerical approach for groundwater flow in unsaturated porous media

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SUMMARY

In this article, a computational tool to simulate groundwater flow in variably saturated non-deformable fractured porous media is presented, which includes a conceptual model to obtain analytical expressions of water retention and hydraulic conductivity curves for fractured hard rocks and a numerical algorithm to solve the Richards equation. To calculate effective saturation and relative hydraulic conductivity curves we adopt the Brooks–Corey model assuming fractal laws for both aperture and number of fractures. A standard Galerkin formulation was employed to solve the Richards' equation together with a Crank–Nicholson scheme with Richardson extrapolation for the time discretization.

The main contribution of this paper is to group an analytical model of the authors with a robust numerical algorithm designed to solve adequately the highly non-linear Richards' equation generating a tool for porous media engineering.

KEY WORDS: flow in porous media; variably saturated flow; constitutive models; finite elements

INTRODUCTION

Simulation of groundwater flow in unsaturated fractured rocks is of interest to many active research areas such as the deep geological disposal of radioactive waste. Deep disposal in crystalline rocks is considered to be an effective means for isolating radioactive waste. However, groundwater migration could contribute to the return of radionuclides to the biosphere. Thus, simulation of groundwater flow provides a useful tool to establish long-term safety of potential disposal sites.

Two possible modelling approaches to deal with flow in fractured media are discrete fracture and continuum models. Even a combination of both [1] could be employed. The first approach

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is based on an explicit description of groundwater flow in individual fractures. This method is computationally expensive and requires a detailed knowledge of geometric properties and spatial distribution of fractures. In the continuum approach the fracture network and the rock matrix are considered as an equivalent porous medium. This method is computationally less expensive but its accuracy largely depends on the accuracy of the constitutive relations of the equivalent porous medium. In the present study the continuum approach is adopted to simulate groundwater flow in unsaturated fractured hard rocks.

As it is difficult to directly measure constitutive relations for a fracture network in the field, these relations have been determined from numerical simulations of steady-state unsaturated flow in two-dimensional fracture networks [2]. Use of numerical simulation to determine large-scale effective constitutive relations for unsaturated flow in porous media has also been reported [3, 4]. This methodology requires one simulation for each point of the water retention curves.

In this work, constitutive relationships are described using a new model developed by the authors, and closed analytical expressions are derived. As a consequence, the simulation code results computationally efficient, because it is not necessary to make several simulations to obtain the water retention curves.

Groundwater flow is assumed to obey Richards' equation. Under unsaturated conditions it is a highly non-linear parabolic equation, but it becomes elliptic and linear when the porous media is fully saturated. Analytical solutions are not possible except for special cases. In the last three decades many numerical methods have been developed to solve this equation, with different results. In general terms, numerical methods to solve the 'h-based' form are the most common because they can be used for saturated and unsaturated soils. However, these models often suffer from mass balance problems and unacceptable time step limitations [5]. The approach used in this paper has demonstrated to be free of these problems [6].

Richards' equation is approximated by using a finite element method for the spatial discretization combined with a third-order accurate algorithm for time approximation, based on the Crank–Nicholson scheme. A Picard iteration method is used to deal with non-linear terms. The algorithm is implemented in two-dimensional domains using unstructured triangular meshes. To illustrate the performance and utility of the proposed algorithm, a water infiltration test in a fractured rock is analysed.

Although the constitutive model is being fully presented in a paper already sent to Hydrogeology Journal, and the numerical strategy in Reference [6], just an abstract is presented for the sake of completeness.

The main contribution of this paper is to group an analytical model of the authors to obtain water retention curves in a non-deformable fractured porous medium with a robust numerical algorithm designed to solve adequately Richards' equation generating a practical tool for porous media engineering.

GOVERNING EQUATIONS

Richards' equation

As mentioned above, groundwater flow through unsaturated fractured rocks is described by the 'h-based' Richards' equation [7]. In our study this equation was stated in terms of the hydraulic head H within a bidimensional domain Ω with boundary $\partial\Omega = \Gamma^D \cup \Gamma^N$ and $\Gamma^D \cap \Gamma^N = \emptyset$

$$C(H)\frac{\partial H}{\partial t} + \nabla \cdot [\mathbf{K}(H)\nabla H] = 0 \quad \mathbf{x} \in \Omega \tag{1}$$

$$\begin{aligned} H(\mathbf{x}, t) &= H^*(\mathbf{x}, t), \quad \mathbf{x} \in \Gamma^D \\ -K(H)\nabla H \cdot \upsilon &= q^*(\mathbf{x}, t), \quad \mathbf{x} \in \Gamma^N \\ H(\mathbf{x}, 0) &= H^0(\mathbf{x}), \quad \mathbf{x} \in \Omega \end{aligned} \tag{2}$$

where $C(H) = \partial\theta/\partial H$ is the moisture capacity, θ being the water content, $\mathbf{K}(H)$ the hydraulic conductivity tensor, and t the time variable. H^* is the prescribed value of hydraulic head over Γ^D, υ is the unit outer normal, q^* denotes the specified values of normal component of flow at Γ^N and H^0 is the initial condition. Hydraulic head H is related to pressure head h by

$$H = h + z \tag{3}$$

where z is the vertical dimension.

As already stated in the introduction, this is a highly non-linear equation, and hence the choice of the numerical method plays a key role in the approximation of the problem.

MODELS AND APPROXIMATIONS

Constitutive model

To solve Equation (1), appropriate constitutive relations between water content θ and H and between K and H are necessary.

To compute the effective saturation and hydraulic conductivity curves of the fractured medium, a specific model has been developed. Although a complete derivation of the equations will appear in Reference [8], currently in review process, a summary is presented here to show the complete analytical expressions for effective saturation and relative hydraulic conductivity, just for the sake of completeness.

Common approaches for deriving hydraulic conductivity curves rely on Mualem or Bourdine models [9, 10]. These models predict the relative hydraulic conductivity curves from knowledge of the water content curves. Tensor $\mathbf{K}(H)$ will be modelled as $\mathbf{K}(H) = \mathbf{K}_s K_r(H)$ where $\mathbf{K}_s$ is the saturated hydraulic conductivity tensor and $K_r(H)$ is a relative hydraulic conductivity function. For unsaturated soils Van-Genuchten's model is widely accepted, but in the case of fractured rocks a constitutive model has to be derived.

A known method to deal with groundwater flow modelling in fractured rocks is the continuum approach. This method considers mean values of both problem variables and physical properties defined in a reference elementary volume (REV). A constitutive model (i.e. relations between capillary pressure, saturation and relative permeability) is necessary to represent adequately physical processes. Accuracy of the modelling results is largely determined by the accuracy of these constitutive relations that characterize flow processes at a subgrid scale (orders of 10–100 m) [2].

In the present approach the hydraulic conductivity of a fractured medium is obtained considering a fracture network as an equivalent continuum medium and then describing the mean properties of fractures in a macroscopic framework. The macroscopic scale is related to the REV dimensions where each fracture is conceptualized as a porous medium of granular structure. To make the approach valid, the REV size must be both larger than the scale of microscopic heterogeneities and smaller than the scale of the domain being studied.

The connectivity among fractures determines the flow description through the REV. In this work the concept of active and inactive fractures [11] is adopted. Only a fraction of connected fractures, called *active fractures*, contributes to groundwater flow, while the remaining fractures are inactive. The number of active fractures in an unsaturated system depends on the pressure head and the capillarity properties of the fracture network [11]. All connected fractures are active if the fracture system is fully saturated and all fractures are inactive if the system is at residual saturation. This model assumes a preferential flux dominated by gravity, similar to the *fingering flux* observed in unsaturated porous media.

The hydraulic conductivity of a fractured medium is obtained from the mass flow conservation in the REV at any time t. The mass flow is computed from the contribution of all active fractures, assuming that the Buckingham–Darcy law [12, 13] is valid.

Under the hypothesis of an isotropic medium, using the Brooks–Corey model [6], and assuming fractal distributions for the number and aperture of fractures, while the total number of fractures are also supposed to obey a fractal law [15], closed-form analytical expressions for the effective saturation of the fractured medium S_{EMF} and the relative hydraulic conductivity K_{RMF} can be obtained.

If D $(1 \leqslant D \leqslant 3)$ is the fractal dimension for the number of fractures, and d the fractal dimension for the fracture aperture, defining q as $q = D - 1/d$, for $q \neq 1$, S_{EMF} can be written as

$$S_{\mathrm{EMF}}(h) = \begin{cases} 1, & h \geqslant h_2 \\ A_1(\beta|h|)^{-\lambda(\gamma+1)} + A_2(\beta|h|)^{-1+q} + A_3, & h_1 < h < h_2 \\ A_4(\beta|h|)^{-\lambda(\gamma+1)}, & h \leqslant h_1 \end{cases} \tag{4}$$

where $\beta = \rho_{\mathrm{w}} g / 2\sigma$, $h_1 = -(\beta b_1)^{-1}$, $h_2 = -(\beta b_2)^{-1}$,

$$A_1 = \frac{1-q}{1-q-\lambda(\gamma+1)} \frac{b_2^{1-q-\lambda(\gamma+1)}}{b_2^{1-q} - b_1^{1-q}}$$

$$A_2 = \frac{-\lambda(\gamma+1)}{1-q-\lambda(\gamma+1)} \frac{1}{b_2^{1-q} - b_1^{1-q}}$$

$$A_3 = \frac{-b_1^{1-q}}{b_2^{1-q} - b_1^{1-q}}$$

and

$$A_4 = \frac{1-q}{1-q-\lambda(\gamma+1)} \frac{b_2^{1-q-\lambda(\gamma+1)} - b_1^{1-q-\lambda(\gamma+1)}}{b_2^{1-q} - b_1^{1-q}}$$

For the case $q = 1$, S_{EMF} takes the form

$$S_{\mathrm{EMF}}(h) = \begin{cases} 1, & h \geqslant h_2 \\ A_1(\beta|h|)^{-\lambda(\gamma+1)} + A_2 \ln(b_1\beta|h|) + A_3, & h_1 < h < h_2 \\ A_4(\beta|h|)^{-\lambda(\gamma+1)}, & h \leqslant h_1 \end{cases} \tag{5}$$

where $A_1 = -b_2^{-\lambda(\gamma+1)}/\lambda(\gamma+1)\ln(b_1/b_2)$, $A_2 = -[\ln(b_1/b_2)]^{-1}$, $A_3 = [\lambda(\gamma+1)\ln(b_1/b_2)]^{-1}$ and $A_4 = b_2^{-\lambda(\gamma+1)} - b_1^{-\lambda(\gamma+1)}/\lambda(\gamma+1)\ln(b_1/b_2)$.

The hydraulic conductivity of the fractured medium is $K_{\mathrm{MF}}(h) = K_{\mathrm{SMF}} K_{\mathrm{RMF}}(h)$, where K_{SMF} is the saturated hydraulic conductivity, and the relative hydraulic conductivity for a fractured rock $K_{\mathrm{RMF}}(h)$ can be written as

$$K_{\mathrm{RMF}}(h) = \begin{cases} 1, & h \geqslant h_2 \\ B_1(\beta|h|)^{-2-(3+\gamma)\lambda} + B_2(\beta|h|)^{-3+q} + B_3, & h_1 < h < h_2 \\ B_4(\beta|h|)^{-2-(3+\gamma)\lambda}, & h \leqslant h_1 \end{cases} \tag{6}$$

where

$$B_1 = \frac{3-q}{1-q-(3+\gamma)\lambda} \frac{b_2^{1-q-(3+\gamma)\lambda}}{b_2^{3-q} - b_1^{3-q}}$$

$$B_2 = \frac{-(3+\gamma)\lambda - 2}{1-q-(3+\gamma)\lambda} \frac{1}{b_2^{3-q} - b_1^{3-q}}$$

$$B_3 = \frac{-b_1^{3-q}}{b_2^{3-q} - b_1^{3-q}}$$

and

$$B_4 = \frac{3-q}{1-q-(3+\gamma)\lambda} \frac{b_2^{1-q-(3+\gamma)\lambda} - b_1^{1-q-(3+\gamma)\lambda}}{b_2^{3-q} - b_1^{3-q}}$$

In these expressions, apertures in the range $b_1 \leqslant b \leqslant b_2$ are considered, h is the pressure head, $\alpha(b)$ and λ are parameters of the Brooks–Corey model, g is gravity acceleration, ρ_{w} the water density, γ is a positive constant depending on properties of the fracture network [11], and σ is the water surface tension.

Numerical approximation

A finite element procedure to solve the original differential problem (1) is adopted. The reader can find a complete detail of the weak form in Reference [6]. The Galerkin formulation applied yields the system

$$\mathbf{M}(\mathbf{H})\frac{\partial \mathbf{H}}{\partial t} + \mathbf{A}(\mathbf{H})\mathbf{H} = \mathbf{B} \tag{7}$$

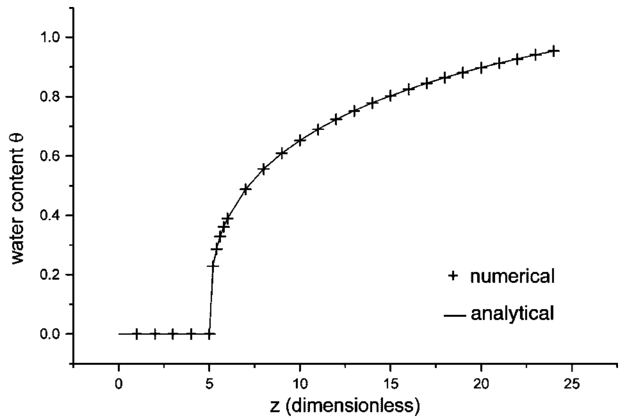

Figure 1. Numerical and analytical solutions of the infiltration test designed by Ross and Parlange [16].

where **H** is the vector of heads at mesh nodal points, **M** and **A** are mass and stiffness matrices, respectively, while vector **B** includes sinks and sources. These non-linear integrals are evaluated using a second-order Gaussian quadrature.

System (7) is approximated in time using two-time step finite differences. A Crank–Nicholson scheme using a fractional step with Richardson's extrapolation was adopted. The numerical solution at time $n+1$ is obtained as

$$H^{n+1} = \frac{H^{n+1}_{\mathrm{CN},r} - r^{-s} H^{n+1}_{\mathrm{CN},1}}{1 - r^{-s}} + O(\Delta t^{s+1}) \tag{8}$$

where $H^{n+1}_{\mathrm{CN},1}$ and $H^{n+1}_{\mathrm{CN},r}$ are the numerical solutions at time step $n+1$ using a Crank–Nicholson scheme with time steps Δt and $\Delta t/r$, respectively, s denotes the order of accuracy of time discretization and $1/r$ is the fraction of Δt used for the fractional step strategy. In our case $s=2$, $r=3$, and the extrapolated solution will be third-order accurate. This temporal integration is unconditionally stable for $r=3$ for almost all values of Δt [6].

To preserve second-order accuracy of the Crank–Nicholson scheme the resulting non-linear system of algebraic equations was linearized using a Picard scheme [17].

The iterative procedure starts with $\mathbf{H}^{n+1,0} = \mathbf{H}^n$ and stops whenever

$$2\left[\frac{\|\mathbf{H}^{n+1,j+1} - \mathbf{H}^{n+1,j}\|_2}{\|\mathbf{H}^{n+1,j+1} + \mathbf{H}^{n+1,j}\|_2}\right]^{1/2} \leqslant \delta \tag{9}$$

where superscript j denotes iteration level of Picard scheme and $\|\cdot\|_2$ is the discrete L^2-norm and δ is a prescribed value for numerical error of the Picard method. The system of equations (7) once linearized using this algorithm involves a positive definite matrix and is solved using a squared conjugated gradient solver with a preconditioning based on incomplete lower-upper factorization.

The proposed algorithm is computationally efficient and numerical results were validated using analytical solutions obtained by Ross and Parlange [16]. The agreement between both numerical and analytical solutions is shown in Figure 1.

NUMERICAL EXAMPLE

In this section, the proposed algorithm is used to simulate groundwater infiltration in a fractured rock. The numerical test was designed to show the performance and practicity of the algorithm in variably saturated conditions and a non-deformable fractured medium. Although due to the nature of the problem, it is not possible to compare it with an analytical solution, the result obtained shows a water behaviour according to what is expected. Fracturation data were extracted from research by Liu and Bodvarsson [2] which represents a very low permeability fractured rock. Similar fracture networks have been used by other researchers to study flow and transport properties of fractures [18].

The domain is 20 m wide by 15 m deep. As it is a two-dimensional example, results represent a unitary thickness domain, which is discretized using 2730 triangular elements (1436 nodes).

A hydrostatic state was assumed as initial condition, with a horizontal water table at 13 m below the surface. At time $t = 0$, a constant infiltration rate of 0.864 mm/day was applied to an interval of 10 m located in the left half of the upper boundary. This low value has been selected as corresponding to an arid zone. No-flux conditions were applied to the rest of the domain boundaries.

The hydraulic parameters of the constitutive model used in the present example correspond to a two-dimensional synthetic fractured media designed by Liu and Bodvarsson [2]. The fracture network consists of random vertical and horizontal fractures with an average density in both directions of 2.2 fractures per meter (see Figure 2 taken from Reference [2]). The trace length and aperture of fractures vary from 0.75 to 3.78 m and 6.67×10^{-5} to 4.2×10^{-4} m, respectively.

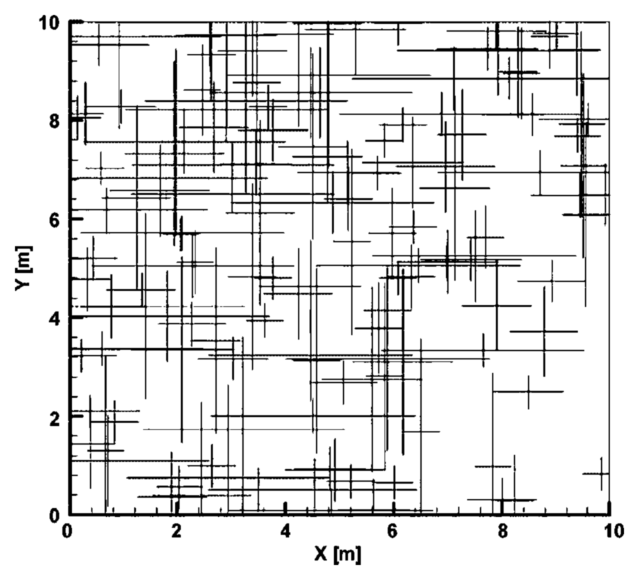

Figure 2. Random-generated fracture network used for the numerical experiment.

Table I. Parameters of Liu–Bodvarsson model.

Parameter	Value
α (cm^{-2})	1.39×10^{-2}
M	0.379
K_s (cm/s)	1.013×10^{-3}
θ_s	7.8×10^{-4}
θ_r	10^{-6}

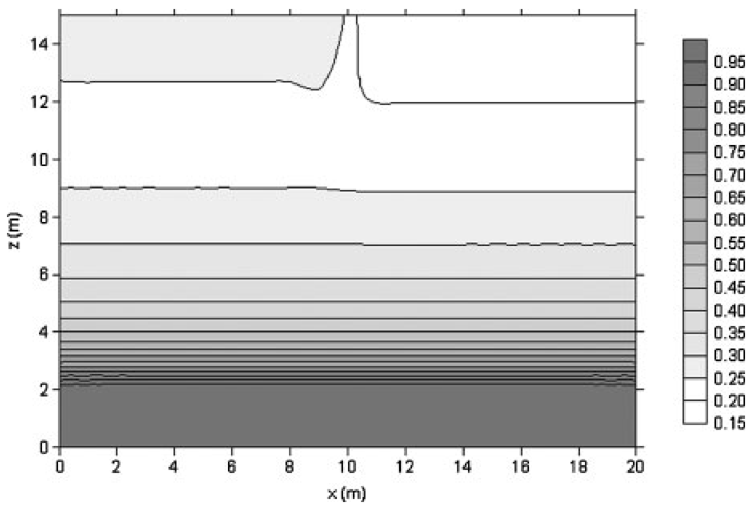

Figure 3. Effective saturation after 6 h of simulation.

The saturated hydraulic conductivity K_s and the saturated water content θ_s for this constitutive model were estimated using the known *cubic law* expressions [19]

$$K_s = \frac{\rho_w g e^3}{12\mu s} \quad \theta_s = \frac{2e}{s} \tag{10}$$

where e is the average aperture; s, the mean distance between two fractures and μ, the dynamic viscosity. The numerical values of these parameters are listed in Table I.

Figures 3–5 show effective saturation S_e profiles calculated after 6, 24 and 96 h of simulation, respectively. As expected in fractured rocks, groundwater infiltrates at a relatively fast rate. Due to this fast infiltration, an elevation of water table levels takes place on the left side of the domain. The shape of pressure head contours in the upper region suggests a horizontal flow from the boundary with infiltration to the right side of the domain where no infiltration is specified. After a simulation of 4 days, the water table elevation in the left boundary can be estimated in 6 m (Figure 5).

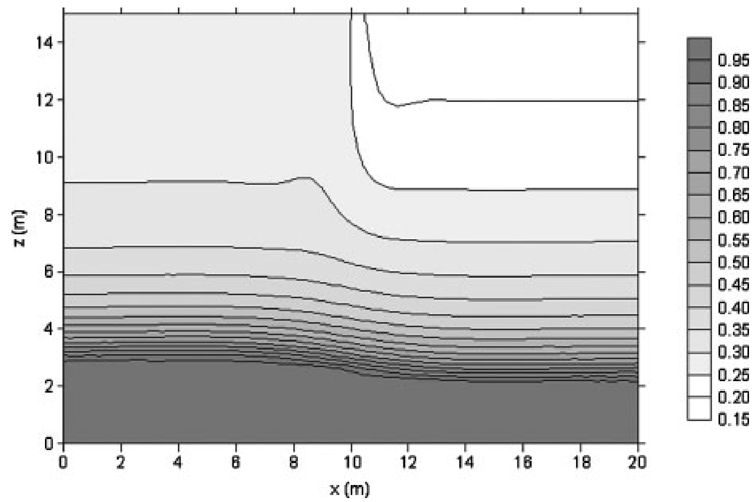

Figure 4. Effective saturation after 24 h of simulation.

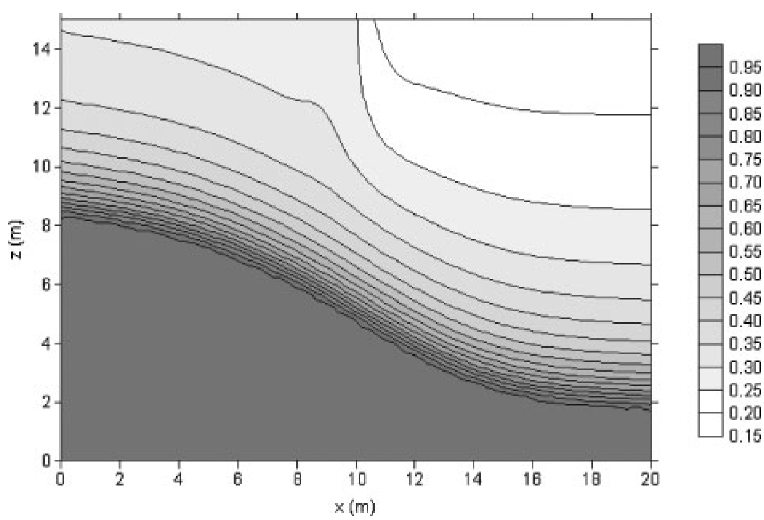

Figure 5. Effective saturation after 96 h of simulation.

Due to the fact that analytical expressions were developed to compute water retention curves, the final solution was obtained after a few minutes of processing in a Pentium IV 500 MHz processor, allowing interactive tasks. There was no need to obtain these curves via numerical simulation. This characteristic shows a high flexibility to compare media with different fracturation parameters, because it can be done just by changing these parameters in the input data.

CONCLUSIONS

In this paper a complete tool to simulate groundwater flow in fractured media is presented. It contains a constitutive model with closed analytical expressions developed for fractured hard rocks, and a careful treatment of the temporal term of Richards Equations, using a third-order scheme, together with a standard Galerkin formulation for the spatial discretization and a Picard algorithm to deal with the non-linear terms.

A two-dimensional non-linear problem of non-saturated fractured medium groundwater flow based on the continuum approach has been simulated in a few minutes of processing in a Pentium IV 500 MHz processor, showing computational efficiency. The analytical expressions obtained to describe appropriately the water retention curves gives the code a good flexibility to change fracturation parameters and then compare different media. The numerical approximation involves the solution of Richards' equation using a finite element technique along with a new constitutive model for characterizing fractured media. An accurate third-order approximation on time derivatives was used, and no convergence problems were observed. From the numerical example we can conclude that the algorithm proposed is a useful tool for predicting moist distribution and for studying groundwater infiltration in fractured media under variably saturated conditions.

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REFERENCES

1. Martínez-Landa L, Carrera J. An analysis of hydraulic conductivity scale effects in granite (Full-scale Engineered Barrier Experiment (FEBEX), Grimsel, Switzerland). *Water Resources Research* 2005; **41**(W03006).
2. Liu H-H, Bodvarsson GS. Constitutive relations for unsaturated flow in a fracture network. *Journal of Hydrology* 2001; **252**:116–125.
3. Desbarats AJ. Scaling of constitutive relationships in unsaturated heterogeneous media: a numerical investigation. *Water Resources Research* 1998; **34**(6):1427–1436.
4. Kueper BH, McWhorter DB. The use of macroscopic percolation theory to construct large-scale capillary pressure curves. *Water Resources Research* 1992; **28**(9):2425–2436.
5. Celia MA, Bouloutas ET, Zarba RL. A general mass-conservative numerical solution for the unsaturated flow equation. *Water Resources Research* 1990; **26**:1483–1496.
6. Guarracino L, Quintana F. A third order accurate time scheme for variably saturated groundwater flow modeling. *Communications in Numerical Methods in Engineering* 2004; **20**(5):379–389.
7. Richards L. Capillary conduction of liquids through porous media. *Physics* 1931; **1**:318–333.
8. Guarracino L, Quintana F, Millán D. A constitutive model for water flow in unsaturated fractured hard rocks. *Hydrogeology Journal* (Manuscript Number: HJ-2004-0076), submitted.
9. Mualem Y. A new model for predicting the hydraulic conductivity of unsaturated porous media. *Water Resources Research* 1976; **12**:513–522.
10. Bourdine NT. Relative permeability calculations from pore-size distribution data. *Transactions of the American Institute of Mining, Metallurgical and Petroleum Engineers* 1953; **198**:71–77.
11. Liu HH, Dougthy C, Bodvarsson GS. An active fracture model for unsaturated flow and transport in fractured rocks. *Water Resources Research* 1998; **34**:2633–2646.
12. Buckingham E. Studies in the movement of soil moisture. *Technical Report*, US Department of Agriculture, Washington, DC, 1907.
13. Bear J. *Dynamics of Fluids on Porous Media*. American Elsevier Publishing: New York, 1972, ISBN 0-486-65675-6.
14. Brooks RH, Corey AT. Hydraulic properties of porous media. *Hydrology*, *Paper No. 3*, Colorado State University, Fort Collins, 1964.

15. Renshaw CE. Fracture Spatial Density and the anisotropic connectivity of fracture networks. In *Dynamics of Fluids in Fractured Rocks*, Faybishenko B, Witherspoon PA, Benson SM (eds), Geophysical monograph, vol. 122. American Geophysical Union, 2000; 203–211.
16. Ross PJ, Parlange JY. Comparing exact and numerical solutions for Richards' equation for one-dimensional infiltration and drainage. *Soil Science* 1994; **157**:341–344.
17. Paniconi C, Aldama AA, Wood EF. Numerical evaluation of iterative and non-iterative methods for the solution of the non-linear Richards equation. *Water Resources Research* 1991; **27**:1147–1163.
18. Smith L, Scwartz FW. Solute transport through fracture networks. In *Flow and Contaminant Transport in Fractured Rock*, Bear J, Tsang CF, De Marsily G (eds). Academic Press: San Diego, 1993.
19. Bear J, Berkowitz B. Groundwater flow and pollution in fractured rock aquifers. In *Developments in Hydraulic Engineering*, Novak IP (ed.), vol. 4. Elsevier: Amsterdam, 1987.

