LBL-31975
UC-814

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

EARTH SCIENCES DIVISION

Presented at the Third International High-Level Radioactive Waste Managment Conference, Las Vegas, Nevada, April 13-16, 1992, and to be published in the Proceedings

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Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098

LBL--31975

DE92 017022

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This work was carried out under U.S. Department of Energy Contract No. DE-AC03-76SF00098, administered by the DOE Nevada Office, in cooperation with the United States Geological Survey, Denver.

SEMI-ANALYTICAL TREATMENT OF FRACTURE/MATRIX FLOW IN A DUAL-POROSITY SIMULATOR FOR UNSATURATED FRACTURED ROCK MASSES

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ABSTRACT

A semi-analytical dual-porosity simulator for unsaturated flow in fractured rock masses has been developed. Fluid flow between the fracture network and the matrix blocks is described by analytical expressions that have been derived from approximate solutions to the imbibition equation. These expressions have been programmed into the unsaturated flow simulator, TOUGH, as a source/sink term. Flow processes are then simulated using only fracture elements in the computational grid. The modified code is used to simulate flow along single fractures, and infiltration into pervasively fractured formations.

INTRODUCTION

A potential site for an underground radioactive waste repository is in Nevada at Yucca Mountain, in a region consisting of highly-fractured, volcanic tuff.[1] As part of the process of characterizing the site for the purposes of determining its suitability for a repository, we have been developing mathematical and computational models for studying the flow of water in unsaturated, fractured rock masses having low matrix permeability. In order to study highly transient infiltration processes that may occur, we need to be able to treat flows in tuffaceous geological units that consist of two intermingled networks of porosity: a (relatively) high-permeability, low storativity fracture network, and low-permeability, high-storativity matrix blocks. We accomplish this by modifying an existing numerical simulator, TOUGH[2], so as to treat flow between the fracture network and matrix blocks by an analytical expression. This modified code can be used to study transient flow processes that may be expected to occur at Yucca Mountain.

DUAL-POROSITY MODELS

For processes which occur on a sufficiently slow time scale, it is often assumed that the fractured rock mass can be treated as an equivalent porous medium, with an effective permeability that is a weighted average of the permeabilities of the fracture network and the matrix blocks.[3] This approach assumes that the matrix blocks are always in local equilibrium with their surrounding fractures; it is therefore capable of simulating processes that occur slowly enough that pressure equilibrium can be achieved between the fractures and matrix blocks. For highly-transient processes, such as the infiltration that would occur after a precipitation event, the "dual-porosity" nature of the medium must be accounted for. In a dual-porosity medium, the fractures provide most of the high permeability of the rock mass, whereas most of the fluid storage takes place in the relatively low-permeability matrix blocks. The complex behavior of dual-porosity systems arises from the fact that there will be different time scales corresponding to diffusion in the fracture network and in the matrix blocks.

The most commonly used conceptual model of a dual-porosity system assumes the existence of two overlapping continua, the fracture continuum and the matrix continuum. Flow is assumed to take place not only through the fractures, but also between the fractures and the matrix.[4,5] The traditional method of simulating processes in such systems involves explicit discretization of both the fracture continuum and the matrix blocks.[6] Simulations using this approach may require an enormously large number of computational grid blocks for each matrix block. For example, if we discretize a cubical matrix block of side L into smaller, cubical grid blocks, of size, say, L/5, this will lead to $5^3 = 125$ grid blocks in each matrix block. A more efficient approach is the MINC[7] method, in which the matrix block is discretized into nested elements, thus treating flow within each matrix block as being mathematically one-dimensional. We have found that accurate treatment of transient effects with the MINC method requires that the representative matrix block associated with each computational cell of the fracture continuum must itself be broken up into about ten nested grid blocks. Hence simulation of transient processes will require roughly ten times the number of computational cells needed for quasi-steady-state simulations. Since the CPU time required by most numerical simulators grows at least as fast as the number of computational cells, simulation of large-scale transient processes using traditional dual-porosity simulators becomes computationally burdensome.

We have taken the approach of incorporating into a numerical simulator an analytical expression[8,9] for absorption of water into matrix blocks, which then plays the role of a source/sink coupling term for the fractures. A similar treat-

ment for single-phase fluid flow and heat transfer has been taken by Pruess and Wu.[10] This approach is in the spirit of the MINC method, since it assumes that the fractures surrounding each individual matrix block are in local equilibrium, and so imbibition into the matrix block commences simultaneously from its entire outer boundary. Our analytical expression accounts for factors such as block geometry, initial saturation, and the hydrological properties of the matrix blocks. Different absorption expressions have been developed for media which have relative permeability and capillary pressure curves of the van Genuchten-Mualem or Brooks-Corey type. The accuracy of these interaction terms have been verified through numerical simulations of imbibition into single matrix blocks of various shapes and sizes.[9] For either form of the characteristic curves, evaluation of the fracture/matrix flow coupling term requires an insignificant amount of CPU time. The computational meshes used in our simulations then consist only of "fracture elements", whose permeability, porosity, and other properties are those of the fracture system, averaged over a suitably large representative elementary volume (REV[11]). The matrix blocks are not explicitly discretized or represented in the computational mesh, but are accounted for through the source/sink coupling term. The only geometrical properties of the matrix blocks that are required as input to the simulations are their volumes and their surface areas. Flow from the fractures into the matrix blocks at any given location is assumed to begin when the liquid saturation in the fractures at that location reaches some nominal value which is taken to signal the arrival of the liquid front. After this time, the flux of water into the matrix block is calculated from our analytical expressions, as a function of the matrix block properties, initial saturation, and elapsed time since the start of imbibition into that particular block.

FRACTURE/MATRIX FLOW EXPRESSIONS

In a large-scale flow process occurring in an unsaturated dual-porosity medium, the saturations and pressures will vary with time in both the fractures and the matrix blocks. However, due to the much larger permeability of the fractures, diffusion of liquid will typically occur much more rapidly in the fractures than in the matrix blocks. Hence, if a liquid saturation front is diffusing through the fracture network, we expect that the time it takes to travel past a single matrix block will be very small compared with the characteristic time of diffusion within that block. This allows us to make the approximation that any given matrix block is surrounded by fractures that are either "ahead of" or "behind" the saturation front in the fracture network. We therefore assume that the boundary conditions for the matrix block, which are provided by the surrounding fractures, are of the step-function type. That is to say, the saturation in the fracture is at its initial value S_i for $t<t_o$, and then abruptly jumps to some higher value, say S_o, for $t>t_o$. In a sense, we have partially uncoupled the problem, which allows us to solve the diffusion equation in the matrix block under boundary conditions that are assumed to be "known".

Hence the basic problem that must be solved in order to develop analytic expressions for the fracture/matrix flow interactions is that of water imbibing into an initially unsaturated matrix block, under the previously-discussed step-function boundary conditions. Under the assumption that the gas phase is infinitely mobile, the flow of liquid water in an unsaturated porous medium can be described by the highly nonlinear Richard's equation:[12]

$$\mathrm{div}\left[\frac{k k_r(\psi)}{\mu\phi}\,\mathrm{grad}\,\psi(x,t)\right] = \frac{\partial S(x,t)}{\partial t}\ . \qquad (1)$$

In eq. (1), ψ represents the pressure potential of the water in the matrix block. It is positive in regions of full saturation, where it is equivalent to the usual (hydrostatic) pressure used in fluid mechanics; it is negative in regions of partial saturation. The saturation S represents the fraction of pore space that is filled with water. S and ψ are related through the capillary pressure relation, the precise form of which depends on rock type (see below). The parameter k is the permeability of the matrix block under fully-saturated conditions, μ is the viscosity of the pore water, and ϕ is the porosity of the matrix block. $k_r(\psi)$ is the dimensionless relative permeability function, which quantifies the decrease in the permeability to water due to the fact that some of the pores are occupied by air; it is typically a strongly increasing function of S.

There are various assumptions and simplifications inherent in eq. (1) which require some discussion. Most rocks and soils are hysteretic with regards to capillary pressure, which means that the $S(\psi)$ relationship depends on whether drainage or imbibition is occurring, and on the past saturation history of the rock. For most of the processes that we are interested in, the saturations vary monotonically, and so hysteresis can be ignored. Hence, we assume that S is a single-valued function of ψ, with no dependence on past values. Eq. (1) also assumes that as the liquid water imbibes into the matrix, it is not impeded by the air that is initially in place. This assumption is known to be correct for flow into an unbounded medium, since the air can escape ahead of the advancing liquid front. For flow that is assumed to be entering a finite-sized matrix block, it is possible that air will be trapped in a pocket at the center of the block; however, this problem will be ignored in the present discussion.

Finally, eq. (1) also neglects gravity, which otherwise would lead to an additional gravitational potential term $\rho g z$ to be added to the pressure potential ψ. Roughly speaking, gravity can be neglected in the early stages of imbibition, when capillary gradients are large relative to the gravitational gradient. At longer times, the capillary gradients have been smoothed out, and the gravitational gradient predominates. For imbibition into a finite-sized block, the relative effects of the these two gradients are quantified by the ratio of the block size to the "sorptive length", which was defined by Philip[13] in terms of the integral of the relative permeability function with respect to ψ. Zimmerman et al.[9] showed that, using hydrological parameters believed to be appropriate for the Topopah Spring welded tuffs at Yucca Mountain,[14] the sorptive length is about 8 m. This means that, roughly speaking, gravity can be ignored in any matrix block whose diameter is much less than 8 m. Since fracture spacings in the Topopah Spring unit are thought to be on the order of tens of centime-

ters,[15] we can assume that imbibition into matrix blocks is dominated by capillary forces.

Each rock has its own set of "characteristic functions" that describe the relationships between S, ψ and k_r. Two sets of characteristic functions that are often used in modeling the hydraulic behavior of the volcanic tuffs at Yucca Mountain are those that were proposed by Brooks and Corey,[16] and Mualem[17] and van Genuchten.[18] The van Genuchten-Mualem functions are

$$S(\psi) = S_r + (S_s - S_r)[1 + (\alpha|\psi|)^n]^{-m}, \quad (2a)$$

$$k_r(\psi) = \frac{\{1 - (\alpha|\psi|)^{n-1}[1 + (\alpha|\psi|)^n]^{-m}\}^2}{[1 + (\alpha|\psi|)^n]^{m/2}}, \quad (2b)$$

where α is a scaling parameter that has dimensions of 1/pressure, and m and n are dimensionless parameters that satisfy $m = 1 - 1/n$, $n > 2$.[19] S_r is the residual air saturation, at which the liquid phase becomes immobile, while S_s, which is usually very close to 1.0, is the saturation at which the matric potential goes to zero. The Brooks-Corey characteristic functions involve a parameter α which represents the inverse of the "air-entry pressure", defined so that if $|\psi| < 1/\alpha$, then air cannot enter the rock, so that $S = S_s$ and $k_r = 1$. When $|\psi| > 1/\alpha$, the Brooks-Corey characteristic functions are given by

$$S(\psi) = S_r + (S_s - S_r)|\alpha\psi|^{-n}, \quad (3a)$$

$$k_r(\psi) = |\alpha\psi|^{-(3n+2)}, \quad (3b)$$

where n is some parameter that satisfies $n > 1$.[19] The parameters α and n used in these two sets of characteristic functions (2a,b) and (3a,b) have similar meanings, but are not necessarily equal to each other for a given rock.

Eq. (1) is essentially a diffusion equation, with the conductance and capacitance related to the characteristic functions $k(\psi)$ and $S(\psi)$. The nonlinearity of these characteristic functions renders exact solutions to eq. (1) nearly impossible to obtain, even for simple geometries such as one-dimensional flow into an unbounded region. In order to construct a dual-porosity model that is fairly general, we need expressions for the rate of imbibition into finite, irregularly-shaped matrix blocks. To develop such expressions, we have used the following approach. First, we used the integral method to develop approximate expressions for one-dimensional imbibition into an unbounded formation.[8,20] Next, we extended these solutions to regular geometries such as spherical, cylindrical, or slab-like matrix blocks.[9] Finally, we developed scaling laws that allow us to extend these results to irregularly-shaped blocks, based on knowledge of their volumes and surface areas.[9]

The basic problem of imbibition into a matrix block can be formulated as follows. Consider a matrix block occupying a region of space Ω, with boundary $\partial\Omega$. Initially, the block is

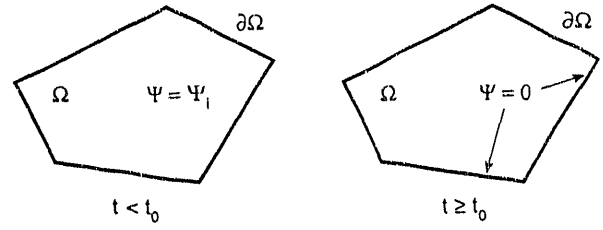

Fig. 1. Schematic diagram of problem to be solved for imbibition into a matrix block.

at some partial saturation S_i, which corresponds to some potential $\psi_i < 0$. At some time t_o the saturation front in the fracture network passes the matrix block, after which the matrix block has the boundary condition $\psi_i = 0$ on the boundary $\partial\Omega$ (see Fig. 1). For both the Mualem-van Genuchten and Brooks-Corey characteristic curves, we have developed fairly accurate solutions[8,20] to this problem for short times, when the problem behaves like imbibition into a semi-infinite medium. Denoting the outer surface area by A, the cumulative volumetric flux Q into the block at early-times, which is the integral of the instantaneous flux, is approximately equal to the following:

Mualem - van Genuchten media:

$$Q = A\left[\frac{2nk\phi(S_s - S_i)^{1+1/n}(t - t_o)}{\alpha(n+1)\mu[m(S_s - S_r)]^{1/n}}\right]^{1/2}; \quad (4a)$$

Brooks-Corey media:

$$Q = A\left[\frac{2k\phi(S_s - S_i)(t - t_o)}{\alpha\mu}\left(1 + \frac{(S_s - S_i)}{2n(S_s - S_r)}\right)\right]^{1/2}. \quad (4b)$$

As an illustration of the accuracy of these solutions, Fig. 2 shows the sorptivity of a Brooks-Corey porous medium, which is defined by $S = Q/A\sqrt{(t - t_o)}$ (for small times), as predicted by eq. (4b) and by numerical solution to the governing equation (1). The approximate solution is very accurate over the entire range of initial saturations, and over the entire range of permissable values of n.

Eqs. (4a,b) show that, for small times, the cumulative flux is equal to $SA\sqrt{(t - t_o)}$. The total flux into the block, at sufficiently long times after the arrival of the saturation front in the adjacent fractures, will be $Q_\infty = \phi V(S_s - S_i)$. Hence the fractional uptake in the blocks, defined by Q/Q_∞, will initially be equal to $SA\sqrt{(t - t_o)}/\phi V(S_s - S_i)$. In other words, at small times, $Q/Q_\infty = \sqrt{\tau}$, where τ is defined by

$$\tau = \left[\frac{S(A/V)}{\phi(S_s - S_i)}\right]^2 (t - t_o). \quad (5)$$

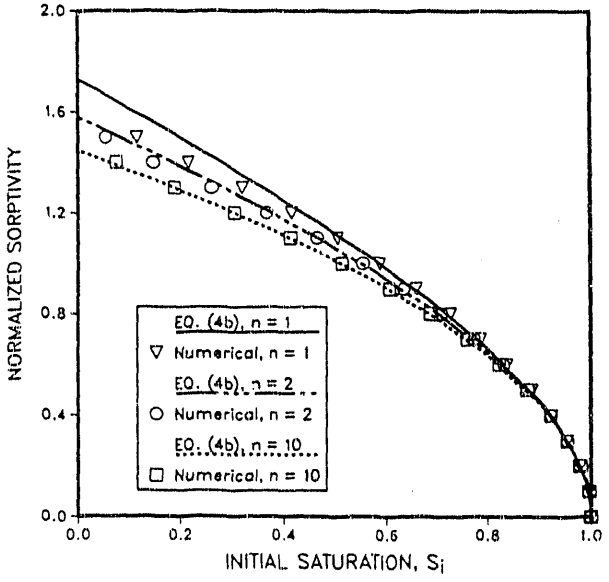

Fig. 2. Normalized sorptivity $S\sqrt{[\alpha\mu/k\phi(S_s - S_i)]}$ of a Brooks-Corey porous medium, as a function of initial saturation, for various values of n. For simplicity, we assume that $S_s = 1.0$ and $S_r = 0$.

We then make the assumption that Q/Q_∞ will be uniquely determined by the variable τ, for all values of t. This implies that the effect of block geometry will be accounted for by the surface-to-volume ratio, A/V. For Mualem-van Genuchten media, we have found that this dependence can be approximated by

$$\frac{Q}{\phi V(S_s - S_i)} = 0.89\sqrt{\tau} - 0.19\tau\,, \qquad (6)$$

where τ is given by eqs. (4a) and (5). Eq. (6) is used until the right-hand-side equals 1, at which time the matrix block is fully saturated; thereafter, the instantaneous flux is zero. This expression has been found to adequately account for the effect of block shape, as well as the effect of initial saturation.[9]

DUAL-POROSITY SIMULATOR

We have implemented our expressions for the fracture/matrix flow as a modification to the TOUGH code, which is an integral finite-difference code that can simulate the flow of liquid water, air and water vapor in porous or fractured media. The TOUGH code contains provisions for sources/sinks of mass and heat, which are calculated in the subroutine QU. The sources/sinks are often used to account for fluid that is injected or withdrawn from a borehole that penetrates one of the computational cells. We have modified this subroutine so as to include a new type of sink, which represents liquid water flowing into the matrix blocks. The magnitude of the instantaneous flux of the sink associated with each computational cell is computed using eqs. (4-6). The subroutine QU calculates a "generation" term G for each cell, at each time step, which represents the average flux for the source/sink over the time interval $t_n \le t \le t_{n+1}$. For fracture/matrix leakage, this generation term is calculated from eq. (6) as

$$G = \frac{Q(\tau_{n+1}) - Q(\tau_n)}{\tau_{n+1} - \tau_n}\,, \qquad (7)$$

where the dimensionless time τ is calculated from eqs. (4a,b) and (5). Leakage from a given fracture element is assumed to begin when the saturation (or capillary pressure) in the fracture reaches some nominal value that is taken to mark the arrival of the saturation front. In the simulations described below, we use 0.90 as the cutoff saturation; further numerical simulations are planned to study the influence of this parameter on the results.

FLOW ALONG A FRACTURE WITH LEAKAGE TO THE MATRIX

One basic problem which has much relevance to understanding the hydrological behavior of the Yucca Mountain tuffaceous rocks is that of water flowing along a fracture, with leakage into the adjacent matrix.[21] Martinez discussed this problem for the case where the fracture is oriented vertically, and the flow downward along the fracture is gravity-driven.[22] In one of Martinez' models, the fracture was assumed to behave as a smooth-walled "slot" of constant aperture, while in another model the fracture was treated as a porous medium with its own characteristic functions. His results showed that the precise details of the hydraulic properties of the fracture were relatively unimportant, and that the absolute permeability was the only property of the fracture that influenced the rate of advance of the water. This result provides some justification for our assumption that the saturation front moves through the fracture network in a piston-like manner. A more detailed mathematical analysis of this problem, including asymptotic results for small and large times, has been given by Nitao and Buscheck.[23]

As an example of a simulation using our dual-porosity code, consider the configuration shown in Fig. 3, with the fracture oriented horizontally. This model would also apply to the early stages of flow along a vertical fracture.[9] Flow into the fracture is driven by the imposed potential at the $y = 0$ boundary. For the matrix blocks, we use the hydrological parameters that have been estimated for the Topopah Spring Member of the Paintbrush Tuff (Miocene) at Yucca Mountain,[15] which are $k = 3.9 \times 10^{-18}\,m^2$, $\alpha = 1.147 \times 10^{-5}\,Pa^{-1}$, $\phi = 0.14$, $S_s = 0.984$, $S_r = 0.318$, and $n = 3.04$. For the fracture we use the same characteristic curves as for the matrix blocks (for illustrative purposes only), but a transmissivity of $8.33 \times 10^{-14}\,m^3$ per unit depth perpendicular to the flow. This transmissivity corresponds[24,25] to a parallel-plate aperture of 100 μm. The fracture is discretized into 14 elements, of successive lengths 1m, 2m, 4m, etc. The temperature is taken to be 20°C. The initial saturation of the matrix blocks is taken to be 0.6765, which corresponds to an initial capillary pressure of -1×10^5 Pa (1 bar).

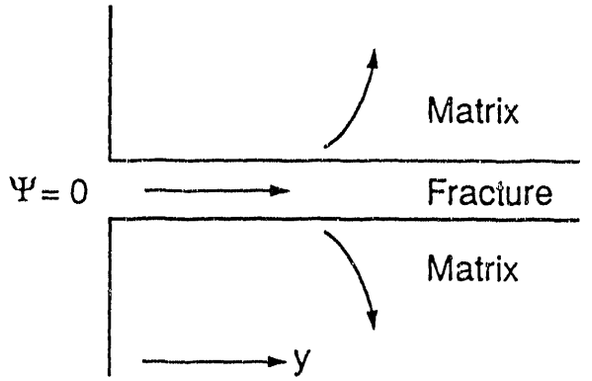

Fig. 3. Schematic diagram of flow along a horizontal fracture, with transverse leakage into the matrix.

We have solved this problem using both the modified version of TOUGH, and also using TOUGH without the source/sink expressions, but with ten grid blocks extending into the matrix adjacent to each fracture element. When using the modified code, we input a very small value of A/V for the matrix blocks, in order to simulate the unbounded region adjacent to the fracture. When solving the problem with explicit discretization of the fracture and matrix regions, the matrix elements must be extended sufficiently far into the the formation so as to effectively simulate a semi-infinite region. The saturation profile in the fracture after an elapsed time of 1×10^3 seconds is shown in Fig. 4, for both methods of calculation. The agreement is excellent, and the decrease in CPU time obtained using the semi-analytical method was 88%.

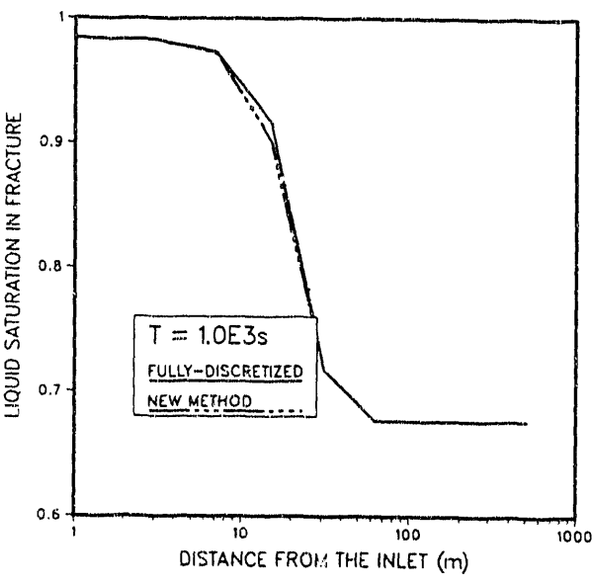

Fig. 4. Saturation profile in the fracture, during flow along a single horizontal fracture. Parameters values used in the simulations are listed in the text.

VERTICAL INFILTRATION INTO A FRACTURED FORMATION

Another hydrological problem of interest for the site characterization process at Yucca Mountain is that of infiltration of liquid water into a pervasively fractured formation, under the influence of both capillary forces and gravitational forces. This infiltration can be modelled as occurring under conditions of constant pressure at the surface, or constant flux.[23] We will consider infiltration to occur under barely-ponded conditions that correspond to a very small positive potential, which we will take to be zero; (The effect of the ponded head h at the surface will be negligible compared to capillarity as long as $\rho g h \ll 1/\alpha$, which in this case will be true as long as the ponded head is no more than a few centimeters).[8] If we assume uniform properties in the horizontal plane, this can be modeled as a one-dimensional problem that is very similar to the leaky-fracture problem discussed above. The only differences in the simulations are the inclusion of a gravitational gradient, and the use of a finite value for A/V, which simulates a finite-size matrix block.

Fig. 5 shows the saturation profile in the fractures, as a function of depth below the surface, after 1×10^3 seconds of infiltration. The effect of gravity is to cause the water to travel much farther than it would have under the influence of capillarity alone (compare Figs. 4 and 5). The agreement between the fully-discretized TOUGH solution and the solution obtained with our new source/sink method is again reasonably close, and the savings in CPU time, which mainly depends on the number of computational blocks used, was again almost 90%. Because the saturation profiles shown in Fig. 5 refer only to the fractures, these profiles do not directly reflect the amount of water that has leaked into the matrix blocks. The total volumetric imbibition into the fractured/porous formation can be measured by examining the instantaneous flux into the first fracture grid block. Comparison of the instantaneous fluxes into the formation also shows very close agreement between the results of the two methods (Fig. 6).

CONCLUSIONS

A semi-analytical dual-porosity model for unsaturated flow in fractured/porous media has been described. An approximate analytical solution for imbibition of liquid water into a matrix block has been incorporated into the numerical simulator TOUGH, to act as a source/sink term for the fracture elements. In its present stage, the analytical treatment of matrix imbibition is applicable to the wetting phase of infiltration processes. The modified code has been tested on the problem of flow along a single horizontal fracture, as well as vertical infiltration into a fractured medium under constant-head boundary conditions. In both cases the new method gives very close agreement with simulations that explicitly discretize the matrix blocks, while yielding a substantial savings in CPU time.

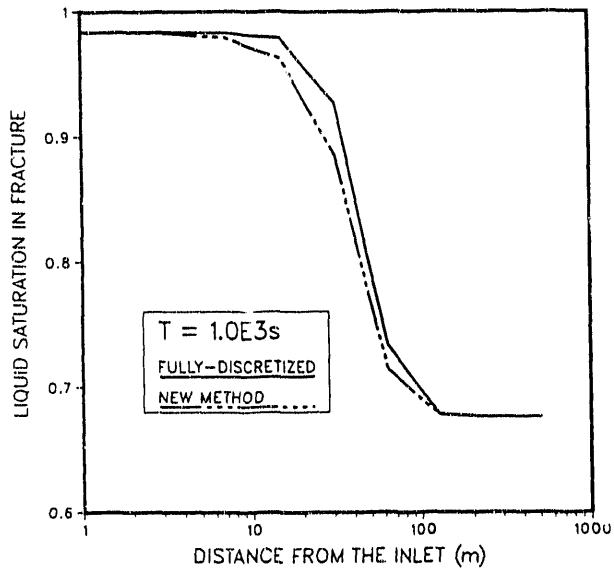

Fig. 5. Saturation profile in the fracture network, during vertical infiltration into a fractured/porous formation. Parameters values used in the simulations are listed in the text.

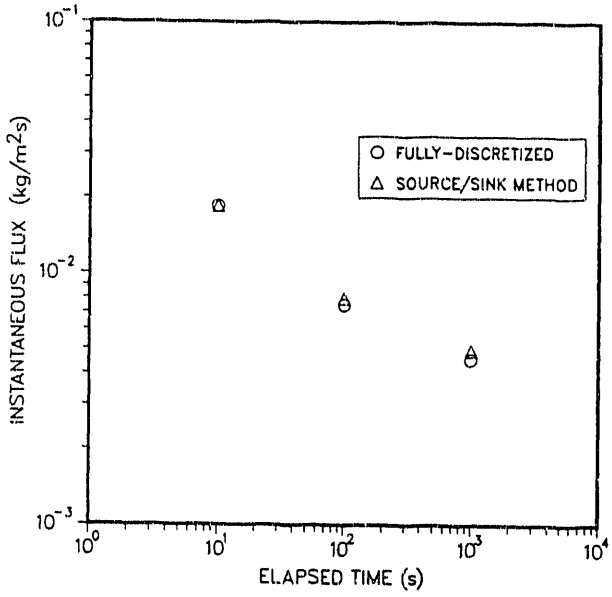

Fig. 6. Instantaneous flux into the fractured/porous formation, for same problem as in Fig. 5.

ACKNOWLEDGEMENTS

This work was carried out under U.S. Department of Energy Contract No. DE-AC03-76SF00098, administered by the DOE Nevada Office, in cooperation with the United States Geological Survey, Denver. The authors thank Gang Chen of LBL for help with the computations, and thank Karsten Pruess and Yvonne Tsang of LBL, and Rick Whitfield and Barney Lewis of the USGS, for reviewing this paper.

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