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Combined Analytical/Numerical Approaches to Solving Fluid Flow Problems in the Unsaturated Zone at Yucca Mountain

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**COMBINED ANALYTICAL/NUMERICAL APPROACHES
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ABSTRACT

Various analytical and numerical approaches are presented for the study of unsaturated flow processes in the vicinity of the Yucca Mountain, Nevada, the proposed site of an underground radioactive waste repository. Approximate analytical methods are used to study absorption of water from a saturated fracture into the adjacent rock. These solutions are incorporated into a numerical simulator as fracture/matrix interaction terms to treat problems such as flow along a fracture with transverse leakage into the matrix. An automatic fracture/matrix mesh generator is described; it allows for more efficient mesh generation for fractured/porous media, and consequently leads to large savings in computational time and cost.

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INTRODUCTION

Yucca Mountain in Nevada is presently being considered as the site of an underground repository for the disposal of high-level radioactive waste.¹ The proposed repository would be located above the water table, in a region of variably-saturated volcanic tuff. As part of the process of characterizing the site for the purposes of determining its suitability for the repository, it is necessary to develop models for studying the flow of water in an unsaturated fractured rock mass with low matrix permeability. The complex fracture geometry, along with other factors, make a purely analytical treatment impractical; at the same time, numerical analysis is constrained by limitations of computational time. Hence, it is desirable to combine both approaches in order to take advantage of the benefits of each. At the Lawrence Berkeley Laboratory we have therefore, in cooperation with the United States Geological Survey at Denver, been developing combined analytical and numerical models to study the hydrological processes that can be expected to occur in the unsaturated zone at Yucca Mountain.

ABSORPTION FROM A FRACTURE

A basic problem that must be solved in order to understand the hydrology of the Yucca Mountain site is that of absorption of water from a fracture into the adjacent partially saturated rock. Under the assumption that the vapor phase is infinitely mobile and at a pressure of one atmosphere, the flow of liquid water in an unsaturated porous medium can be described by the highly nonlinear Richard's equation:²

$$\operatorname{div} [\beta k_r(\psi) \operatorname{grad} \psi] = \frac{\partial S}{\partial t} . \quad (1)$$

The dependent variable ψ in eq. (1) represents the pressure potential of the water in the medium. It is positive in regions of full saturation, and is equivalent to the usual (hydrostatic) pressure used in fluid mechanics. When the medium is less than fully saturated, ψ is negative, and it is sometimes referred to as the matric potential. The saturation S represents the fraction of pore space that is filled with water. β is an hydraulic conductivity parameter that equals $k/\mu\phi$, where k is the permeability of the medium under fully-saturated conditions, μ is the viscosity of the water, and ϕ is the porosity of the medium. k_r is the dimensionless relative permeability, and is typically a strongly increasing function of S . Eq. (1) essentially embodies the principle of conservation of mass for the water, with the left hand side representing the local net influx of water (through a modified form of Darcy's law), and the right hand side representing the change in the volumetric water content.

As written, eq. (1) assumes that the air phase is infinitely mobile, and always at one atmosphere pressure. It also assumes that the porosity does not vary with ψ , which is true to a very high approximation for most rocks. Hysteretic effects, in

which the $S(\psi)$ relationship depends on whether drainage or imbibition is occurring, are also ignored. For the processes that will be discussed in this paper, the saturations always increase, and so hysteresis *per se* does not occur. However, it should be noted that even for monotonic changes in the saturation, the appropriate characteristic curve that must be used is affected by the previous wetting/drying history of the medium. 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 . This is permissible for horizontal flow, or for the initial phase of vertical infiltration, when matric potential gradients may be large compared to gravitational gradients.³

Each porous medium has its own set of characteristic curves that describe the relationships between S , ψ and k_r . One functional form of the characteristic functions that has been found useful in modeling the hydraulic behavior of the volcanic tuffs at Yucca Mountain is that proposed by van Genuchten:⁴

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

$$k_r = \frac{[1 - (\alpha |\psi|)^{n-1} [1 + (\alpha |\psi|)^n]^{-m}]^2}{[1 + (\alpha |\psi|)^n]^{m/2}} , \quad (3)$$

where α is a scaling parameter that has dimensions of 1/pressure, and m and n are dimensionless parameters that satisfy $m = 1 - 1/n$, $n > 1$. The parameter α is in some sense proportional to the average pore diameter in the medium, while n is inversely proportional to the broadness of the pore size distribution. S_r is the residual air saturation, at which the liquid phase becomes immobile, while S_s is the saturation at which the matric potential vanishes.

Consider now the problem of infiltration from a saturated fracture at zero potential (located at $x=0$) into the adjacent semi-infinite formation ($x>0$). In this case, eq. (1) takes the form

$$\frac{\partial}{\partial x} \left[\beta k_r(\psi) \frac{\partial \psi}{\partial x} \right] = \frac{\partial S}{\partial t} . \quad (4)$$

This differential equation must be supplemented by the following boundary and initial conditions:

$$\psi(x, 0) = \psi_i \quad \text{for all } x > 0 , \quad (5)$$

$$\psi(0, t) = 0 \quad \text{for all } t > 0 , \quad (6)$$

$$\lim_{x \rightarrow \infty} \psi(x, t) = \psi_i \quad \text{for all } t > 0. \quad (7)$$

Boundary condition (7) reflects the fact that at any finite time, the effect of the fully-saturated boundary at $x=0$ must become negligible as $x \rightarrow \infty$.

Because of the variation of k_r and S with ψ , eqs. (4-7) represent a highly non-linear problem that is not amenable to standard analytical techniques such as Laplace transforms, Green's functions, etc. Numerous approximate analytical solutions have been derived, with varying degrees of accuracy and ease of implementation. Some of the methods used to obtain these solutions include perturbation techniques,⁵ and variational principles.⁶ Many of these methods are reviewed and discussed by Brutsaert.⁷ Although most of these methods yield results with accuracies that are sufficient for many purposes, they still require some numerical integration of the characteristic functions (2) and (3). Furthermore, they are not applicable to geometries other than the half-space, since they rely on the similarity transformation $\eta = x/\sqrt{t}$.

We have obtained a closed-form approximate solution by using an "integral" technique. This method has been widely used for heat conduction problems,⁸ heat transfer problems with phase change,⁹ and viscous flow problems.¹⁰ Prasad and Römken used a related method to investigate vertical infiltration under time-varying boundary conditions.¹¹ The integral method begins with the choice of a trial solution for the potential profile. The trial solution must satisfy various boundary (or other subsidiary) conditions, and depends on a penetration depth δ whose dependence on time is not known *a priori*. If the profile is substituted into the governing partial differential equation, which is then integrated from 0 to ∞ , the result is an ordinary differential equation that describes the time evolution of δ . The accuracy of the boundary-layer method depends mainly on choosing an appropriate potential profile. Although the potential, strictly speaking, does not reach ψ_i until $x \rightarrow \infty$, for practical purposes it can be considered to equal ψ_i for all $x > \delta$, where δ is the penetration distance.⁵ Since it is convenient to work with the saturation profile instead of the potential profile we require that the trial profile satisfy the conditions $S(0, t) = S_s$, and $S(\delta, t) = S_i$.

The key to choosing a successful profile for this particular problem is insuring that the trial profile has the proper behavior near $x=0$. In order for the flux at the fracture wall to be finite, the potential profile must start off with a finite negative slope, i.e., $\psi(x, t) = -ax + \dots$, where a depends on t , but not on x . To determine the behavior of S in the vicinity of $x=0$, substitute $\psi(x, t) = -ax$ into eq. (2), and then consider the first two terms of the binomial expansion of $[1 + (\alpha|\psi|)^n]^{-m}$, which are $1 - m(\alpha|\psi|)^n$. This leads to $S(x, t) = S_s - bx^n + \dots$, where b depends on t , but not on x , and n is the van Genuchten parameter. The simplest saturation profile that satisfies these criteria is

$$S = S_s - (S_s - S_i)(x/\delta)^n \quad \text{for } 0 < x < \delta,$$

$$S = S_i \quad \text{for } \delta < x < \infty. \quad (8)$$

With the saturation profile given by eq. (8), both sides of eq. (4) can be integrated from $x=0$ to $x=\infty$.¹² The result is a simple differential equation, whose solution yields a relationship between δ as a function of t :

$$\delta = \left[\frac{2(n+1)kt}{\alpha n \mu \phi} \frac{(S_s - S_i)^{-1+1/n}}{[m(S_s - S_r)]^{1/n}} \right]^{1/2}. \quad (9)$$

Since δ grows as \sqrt{t} , and the saturation profile (8) is a function only of x/δ , the approximate solution has the self-similar structure that was shown by Bruce and Klute¹³ to hold regardless of the specific characteristic curves used.

The instantaneous volumetric flux per unit area at the wetted boundary is found by combining eqs. (8) and (9) with Darcy's law:

$$q = \left[\frac{nk\phi(S_s - S_i)^{1+1/n}}{2\alpha(n+1)\mu t [m(S_s - S_r)]^{1/n}} \right]^{1/2}. \quad (10)$$

The cumulative volumetric liquid flux is found by integrating the instantaneous flux over time, which leads to

$$Q = \int_0^t q(t') dt' = \left[\frac{2nk\phi t (S_s - S_i)^{1+1/n}}{\alpha \mu (n+1) [m(S_s - S_r)]^{1/n}} \right]^{1/2}. \quad (11)$$

These results have been extended¹² to the case where the liquid in the fracture is under a positive pressure. The instantaneous flux q that is due to a boundary potential ψ_w is related to the flux q_0 for the case of zero boundary potential by

$$q^2 t = q_0^2 t + k\psi_w \phi (S_s - S_i) / 2\mu. \quad (12)$$

This approximate solution compares well with numerical simulations of absorption rates into the volcanic tuffs found at Yucca Mountain. The Topopah Spring unit is a welded volcanic tuff with an estimated matrix permeability of $3.9 \times 10^{-18} \text{ m}^2$, estimated¹⁴ matrix porosity of 0.14, and estimated van Genuchten parameters of $n=3.04$, $m=0.671$, $S_s=0.984$, $S_r=0.318$, and $\alpha=1.147 \times 10^{-5} \text{ Pa}^{-1}$. Consider a fracture

that is saturated with water at zero potential, with the adjacent formation initially at a saturation of 0.6765. This initial saturation seems to be in the range that has been estimated¹⁵ for the Topopah Spring unit. This problem has been simulated with the TOUGH¹⁶ code, which is an integrated-finite-difference program that models two-phase flow in porous media. The viscosity of water was taken to be 1 cp, or 0.001 kg/m-s. The block matrix was divided into 25 grid blocks, each 0.04 m thick.

Fig. 1 shows the saturation profile for this problem, after an elapsed time of 1×10^7 s (116 days), for both the approximate solution and the numerical simulation. The solution to this problem depends only on the similarity variable x/\sqrt{t} , so the profiles would have the same shapes for any value of time. Since the cumulative flux is proportional to the area under the saturation profile, it is clear that the approximate solution is very accurate in this case. The approximate solution also predicts the location of the wetting front very accurately.

FLOW ALONG A FRACTURE WITH LEAKAGE TO THE MATRIX

Another basic problem which has much relevance to understanding the hydrological behavior of the Yucca Mountain site is that of water flowing along a fracture, with leakage into the adjacent matrix.¹⁷ Martinez¹⁸ discussed this problem for the case where the fracture is oriented vertically, and the flow downward along the fracture is gravity-driven. 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 for this problem; the absolute permeability was the only property of the fracture that influenced the rate of advance of the front. A more detailed mathematical analysis of this problem, including asymptotic results for small and large times, has been given by Nitao and Buscheck.¹⁹

The ultimate goal of this work is to solve large-scale problems using a numerical simulator such as TOUGH, with the approximate expression (10) serving as a source/sink term for the fracture elements, thus alleviating the need for gridding of the matrix blocks. Use of this type of source/sink term will limit simulations to problems where the flow between a fracture element and the adjacent matrix is always in the same direction; problems with oscillatory boundary conditions would require a different form for the source/sink term. As an example of this approach, consider the variation of Martinez' problem shown in Fig. 2, with the fracture oriented horizontally. Flow into the fracture is driven by the imposed potential at the $y=0$ boundary. For simplicity, we use the same characteristic curves as specified above for both the fracture and matrix, but a matrix permeability of 3.9×10^{-20} m², and a fracture permeability of 3.9×10^{-10} m². This fracture permeability corresponds roughly to an aperture of 100 μ m, allowing for tortuosity and contact-area effects. The fracture is discretized

into 10 elements, each 1 m long and 100 μ m thick. Each of these elements has a "sink" term (for which TOUGH already has provisions), the magnitude of which varies with time according to eq. (10). The sink is assumed to be turned on instantaneously when the saturation in the block reaches 0.90, which we consider to represent the arrival of the wetting front. As a comparison, the problem is also solved without the source/sink expressions, but with five matrix elements extending into the matrix adjacent to each fracture element. The matrix elements extend 100 μ m into the formation, which, for the time scale of the problem, is sufficient to simulate a semi-infinite region. The saturation profile in the fracture after an elapsed time of 4×10^3 s is shown in Fig. 3, according to both methods of calculation. The agreement is excellent, and the savings in CPU time (on a CRAY-XMP) obtained using the semi-analytical method was roughly a factor of ten. Note that after 4×10^3 s, about 30% of the fluid that entered the fracture at $y=0$ has leaked off into the formation, so the effect that is being modeled is quite significant.

For the related, but more general, problem of flow along sets of parallel fractures, the source/sink expression for absorption into an infinite medium cannot be used, at least not for times large enough that the wetting fronts moving in from nearby fractures begin to overlap. A source/sink expression for flow into a finite-sized block would be needed for such problems. A reasonably accurate expression for absorption into an arbitrarily-shaped finite-sized block can be found by examining absorption into spherical blocks, and then postulating a scaling-law based on a dimensionless time that involves the ratio of block volume V to surface area A . The result of this analysis²⁰ is that if the dimensionless time τ is defined by

$$\tau = \frac{2(n+1)k(S_s - S_i)^{-m}t}{\alpha n \mu \phi [m(S_s - S_i)]^{1/n} (V/A)^2} , \quad (13)$$

then the cumulative infiltration into the block can be approximated by

$$\frac{Q(\tau)}{\phi V(S_s - S_i)} = 1.79 \sqrt{\tau} - 0.79 \tau . \quad (14)$$

FRACTURED-CONTINUUM PROBLEMS

For some problems it is desirable to treat each fracture explicitly. This will be possible if the number of fractures is not prohibitively large, and if their locations and orientations are known. For such problems, we have developed the fracture/matrix mesh generator program, FMMG.²¹ This program takes as its input the locations, lengths, orientations and apertures of the fractures, and creates a computational mesh that is suitable for use in finite-element or integrated-finite-difference simulators; the

user can specify which type of mesh is desired. The resulting mesh includes both fracture and matrix elements. Currently, FMMG handles only two-dimensional geometries.

The first process that FMMG carries out is to extend each fracture until it intersects either another fracture or the outer boundary of the flow field. These fracture extensions are stipulated to have zero longitudinal transmissivity, although they do permit transverse fluid flow. Their purpose is to assure that the rock is broken up into sets of non-overlapping convex polygons. The next step is to locate these minimal (non-overlapping) polygons. This is done by starting at a node, and traversing the fracture elements in a clockwise direction, always following the path of minimum angle. When the starting node is reached, the path that has been taken defines a polygonal block. The area and center of gravity of this block is then computed; since the block is convex, its center of gravity will always lie inside its boundaries.

The polygonal matrix blocks are then discretized into smaller computational blocks, as in Fig. 4. First, lines are drawn from each corner of the block to the center of gravity, breaking up the block into triangles. Each of these triangles is then broken up into slab-like cells, bounded by lines that are parallel to the outer boundary of the matrix block. The spacing of this set of lines follows a geometric progression, so as to create computational cells of roughly equal area. If the integrated-finite-difference option has been chosen, then the innermost area is not transected by the radial lines, but is left as a single intact block (see Fig. 4). The user can control the number of slabs created in each triangle, as well as the precise spacing of the parallel lines. Finally, the program calculates the area of each cell, the length of the contact line between each cell, and the distance from the center of gravity of each cell to each of its boundaries.

A test of the accuracy of the FMMG gridding approach is shown in Figs. 5 and 6, for the problem of absorption into a polygonal block. Fig. 5 shows the gridding used in the FMMG approach, and the same block discretized by a rectangular grid. The problem was then solved with the TOUGH¹⁶ simulator, using the two gridding methods. Fig. 6 shows the fractional uptake of liquid, plotted against time, for the two simulations. The solution obtained with the FMMG grid agrees very closely with that obtained using the rectangular grid. Since the FMMG grid contained only 11 cells, while the rectangular grid contained 109 cells, there was a substantial saving in CPU time of more than a factor of ten. Since the computational effort required to perform the matrix inversions in TOUGH grows as the square of the number of cells, the savings in CPU time for larger problems can be expected to be even greater than this. It should be noted, however, that this method of gridding can lead to large errors if there is an appreciable saturation gradient along the fractures surrounding a given matrix block.

CONCLUSIONS

A review has been given of various analytical and numerical methods that have been developed to study unsaturated flow at Yucca Mountain, the site of a proposed underground radioactive waste repository. The integral method has been used to derive a closed-form approximation for the influx of water from a saturated fracture into the adjacent formation. Using the hydraulic properties that have been estimated for the Topopah Spring welded tuff, this solution predicts wetting-front locations and infiltration rates that are in close agreement with the results of numerical simulations. The expression for the infiltration rate has been programmed into the numerical simulator TOUGH as a source/sink term, thus eliminating the need for explicitly discretizing the matrix in large-scale simulations. The resulting code was used to solve the problem of flow along a fracture with transverse leakage into the formation. Comparison with a simulation that used both fracture and matrix blocks showed very close agreement with the source/sink method. An automatic fracture/matrix mesh generator (FMMG) has been developed that takes as its input a specified network of fractures, and generates an efficient mesh that is suitable for use with integrated-finite-difference or finite-element codes. This mesh-generator allows a vast decrease in the number of computational elements needed for a simulation, and consequently achieves large savings in CPU time.

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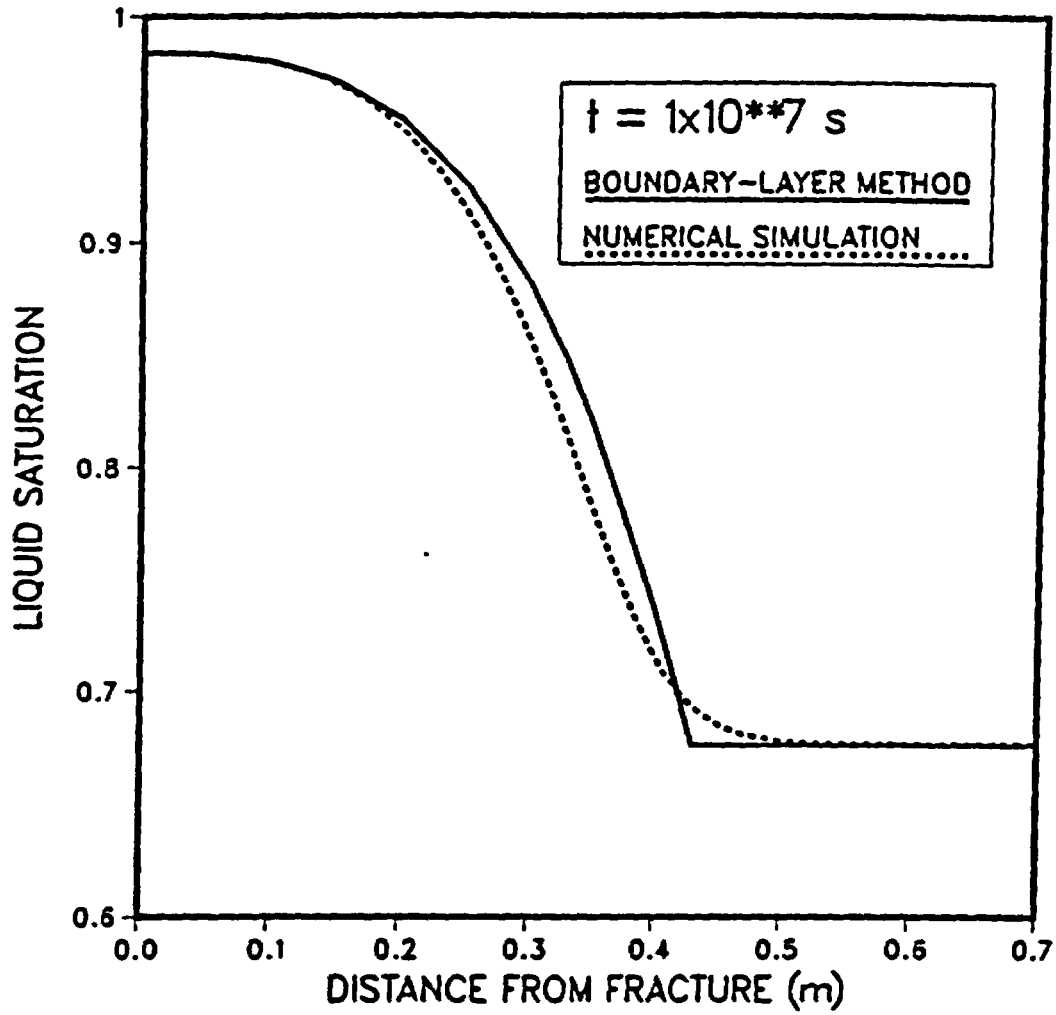


Figure 1. Saturation profiles for one-dimensional absorption in Topopah Spring welded tuff. Physical properties of tuff are listed in text.

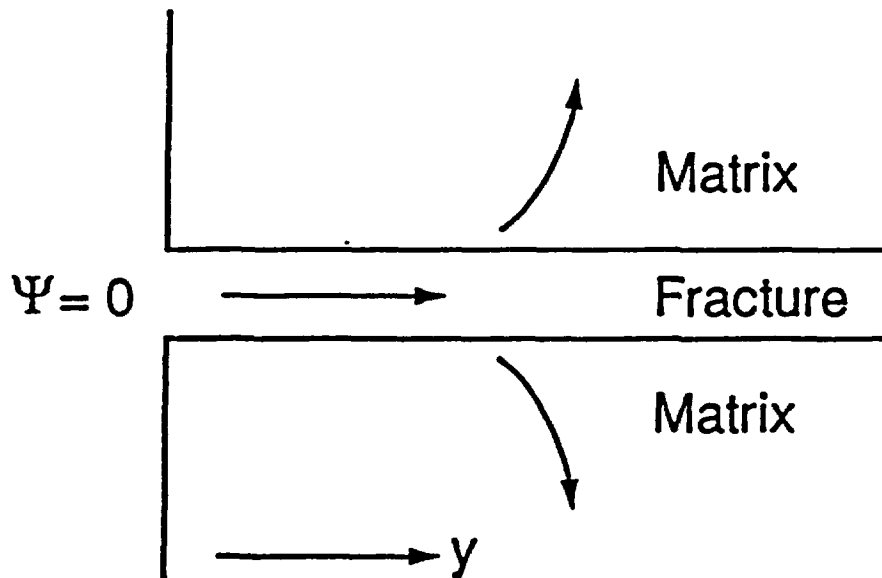


Figure 2. Schematic diagram of the problem of infiltration into a fracture, with transverse leakage into the matrix.

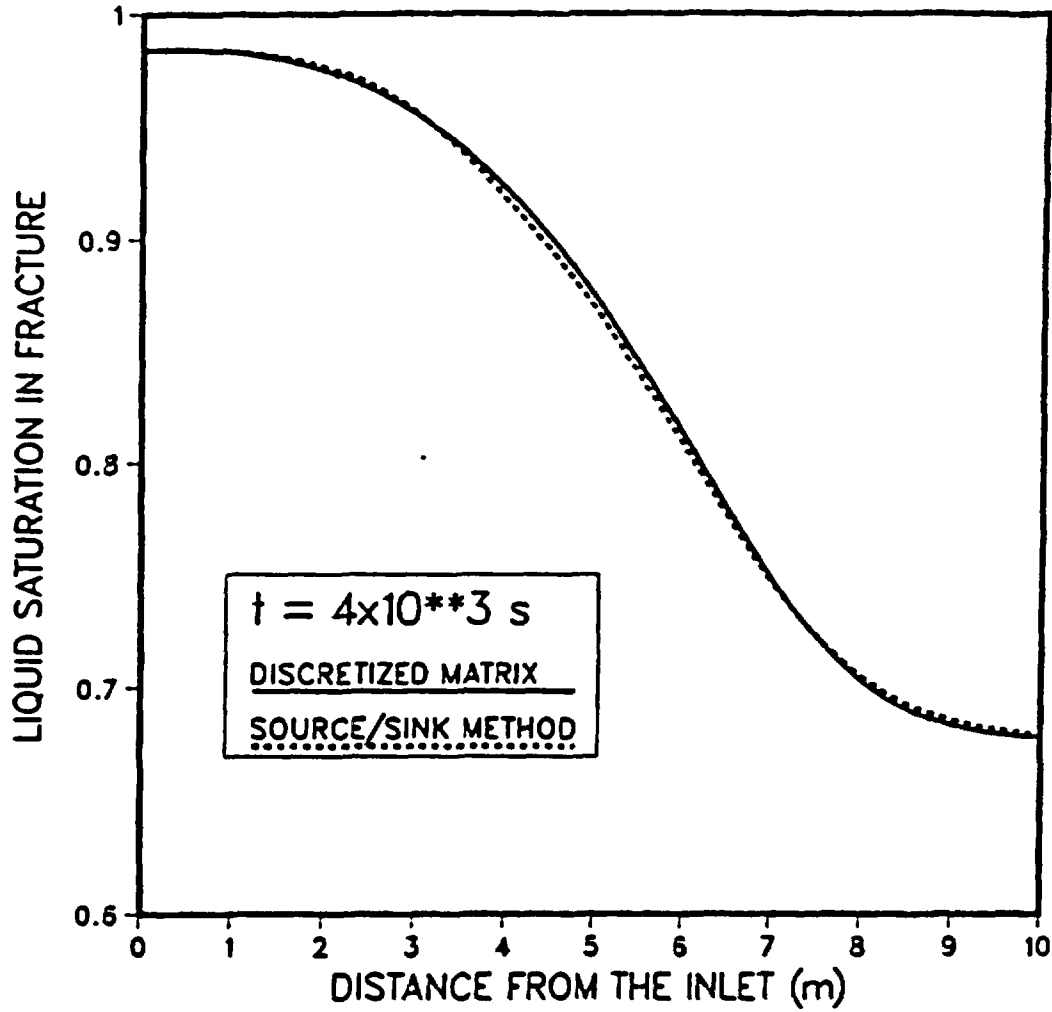


Figure 3. Saturation profile in fracture for flow along fracture with transverse leakage to matrix. Hydraulic properties used in simulations are listed in text.

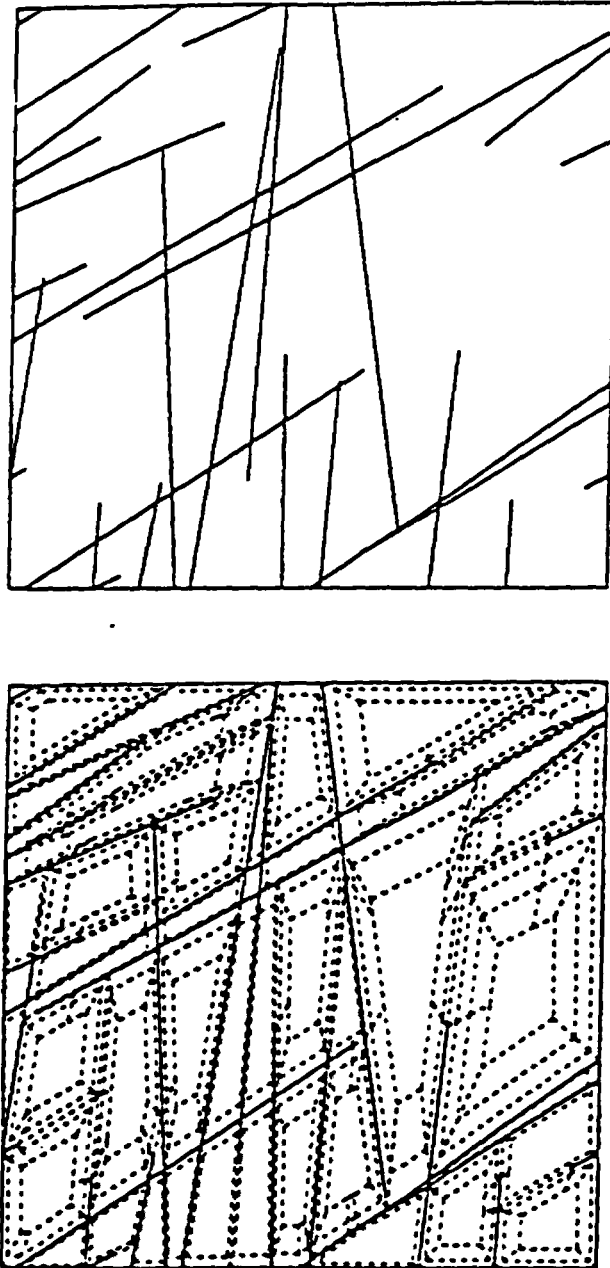


Figure 4. (a) Two-dimensional flow region containing a network of fractures; (b) Discretization of flow region in integrated-finite-difference format, using FMMG.

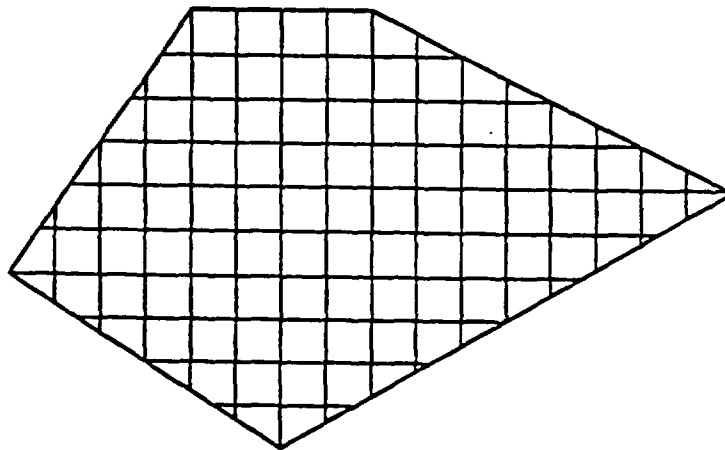
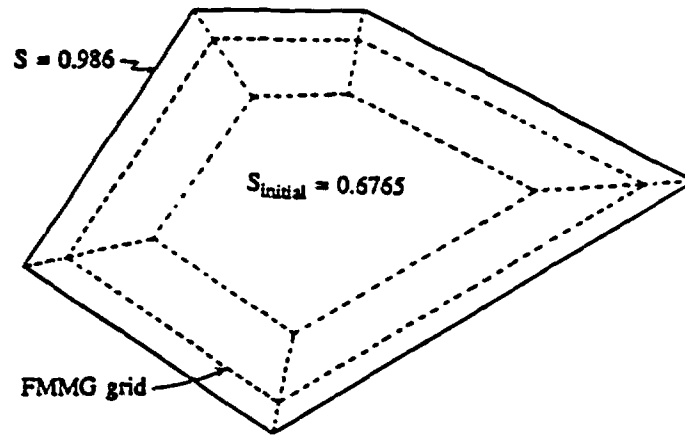


Figure 5. Comparison of the computational grid created by the program FMMG and a rectangular grid, for the problem of liquid absorption into a polygonal block.

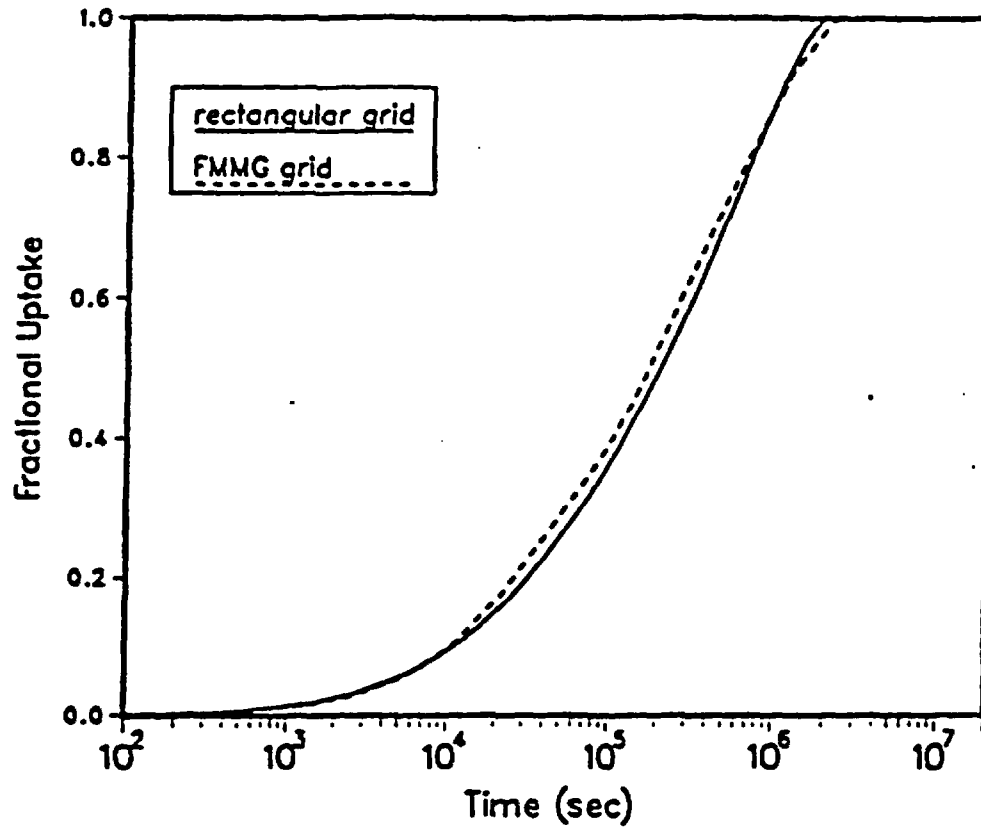


Figure 6. Fractional uptake of liquid for the problem shown in Fig. 4, calculated with TOUGH, using an FMMG grid and a rectangular grid.

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