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Semi-Analytical Solutions for Flow Problems in Unsaturated Porous Media

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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.

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Abstract

Semi-analytical solutions are developed for two unsaturated flow problems that are relevant to characterizing the hydrological behavior of Yucca Mountain, the site of a proposed nuclear waste repository. The "integral" or "boundary-layer" approach is used to find a closed-form approximate solution for absorption of water from a saturated fracture into an unsaturated semi-infinite formation. This solution is then programmed into a numerical code as a source/sink term for fracture elements, and used to study the problem of flow along a fracture with transverse leakage to the rock matrix.

To be presented at the special session on "Multiphase Transport in Porous Media" at the Winter Annual Meeting of the ASME, San Francisco, CA, December 10-15, 1989

Nomenclature

g	gravitational acceleration [m/s^2]
k	absolute permeability [m^2]
k_r	relative permeability
m	van Genuchten parameter, $= 1 - 1/n$
n	van Genuchten parameter for characteristic curves
q	instantaneous liquid flux [m^3/m^{2}s]
Q	cumulative liquid flux [m^3/m^2]
S	liquid saturation
S_i	initial saturation
S_r	residual liquid saturation
S_s	saturation at zero potential
$\hat{S}$	normalized saturation, $= (S - S_r)/(S_s - S_r)$
t	time since start of absorption [s]
x	distance from fracture into formation [m]
y	distance along fracture measured from inlet [m]

Greek letters

α	van Genuchten parameter [ms^2/kg]
β	hydraulic conductivity parameter, $= k/\mu\phi$ [m^3s/kg]
δ	penetration depth of wetting front [m]
η	similarity variable, $= x/\sqrt{t}$
ϕ	porosity
μ	viscosity [kg/ms]
Ω	region occupied by matrix block
$\partial\Omega$	boundary of Ω
ρ	density of water [kg/m^3]
ψ	potential [kg/ms^2]
ψ_i	initial potential [kg/ms^2]
$\hat{\psi}$	normalized potential, $= \alpha\psi$
ζ	integration variable, $= x/\delta$

Introduction

Yucca Mountain in Nevada is presently being considered for the location of an underground repository for the disposal of high-level civilian radioactive waste (U.S. DOE, 1986; Peters and Klavetter, 1988). The proposed repository would be located in the unsaturated zone above the water table, in a region consisting of highly fractured 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 (but nonzero) matrix permeability. The complex 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.

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. Using the usual 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 is described by the highly nonlinear Richard's equation (Hillel, 1980). The nonlinearity stems from the fact that both the capillary pressure and the relative permeability are strongly-varying functions of the water content. Because of this nonlinearity, exact analytical solutions are not feasible, even for simple geometries. We therefore use the "integral method" to derive an approximate solution to the problem of one-dimensional absorption into a half-space. The medium is assumed initially to be at some constant potential, representing a state of partial saturation, with the fractures at the boundary then instantaneously brought to full saturation. The van Genuchten (1980) expressions for the capillary pressure and relative permeability functions are used for the characteristic curves of the porous medium. Explicit and fairly accurate expressions are found for the volumetric flux of liquid into the medium. These

expressions are therefore in a convenient form for incorporation into numerical models as source/sink terms for flow between the fractures and the matrix blocks. The resulting semi-analytical/semi-numerical code is then used to solve the problem of flow along a fracture with transverse leakage to the matrix.

Formulation of the Basic Problem

The flow of water through an unsaturated (also referred to as partially saturated) medium can be described by the following equation (Hillel, 1980; Bear, 1988):

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

The dependent variable ψ in equation (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 capillary pressure or 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 a dimensionless "relative permeability" function, and is typically a strongly increasing function of S. Equation (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, equation (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 and soils.

Hysteretic effects, in which the $S(\psi)$ relationship depends on whether drainage or imbibition is occurring, are also ignored. This causes no difficulty as long as we are concerned only with processes in which the saturation changes monotonically. Finally, equation (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 (Philip, 1970).

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 (1980):

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

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

where α is a scaling parameter that has dimensions of 1/pressure, and m and n are dimensionless parameters that satisfy $m = 1 - 1/n$, $n > 1$. Examples of these functions are plotted in normalized form in Figures 1 and 2, for a range of n values believed to be typical of the Yucca Mountain volcanic tuffs. The normalized potential is defined by $\hat{\psi} = \alpha\psi$, and the normalized saturation as $\hat{S} = (S - S_r)/(S_s - S_r)$. 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. The capillary pressure curve (Figure 1) has a sigmoidal shape that more closely approximates a step function as the pore size distribution narrows and n increases. The quasi-horizontal plateau of the capillary pressure curve, where S varies most rapidly with ψ, occurs at a potential approximately equal to $-1/\alpha$.

A basic problem that we are interested in involves of a block of porous material which is initially at some uniform level of saturation, S_i. Through equation (2), this corresponds to some initial potential ψ_i. In the field, the initial saturation (under equilibrium conditions) will generally vary with depth. At Yucca Mountain, however, the fracture spacing is so small (less than 1 m; Rulon et al., 1986) that any individual matrix block can be considered to be initially at a uniform saturation. At some time $t=0$, the fractures that form the boundary of the block become saturated at zero potential. Since the permeability of the fractures greatly exceeds that of the matrix blocks, it can be assumed that this boundary condition is established instantaneously. If the block occupies a region of space denoted by Ω, with boundary $\partial\Omega$ (see Figure 3), the boundary and initial conditions are

$$\psi(\vec{x}, t=0) = \psi_i \quad \text{for all } \vec{x} \in \Omega \,, \tag{4}$$

$$\psi(\vec{x}, t>0) = 0 \quad \text{for all } \vec{x} \in \partial\Omega \,. \tag{5}$$

For a given block geometry Ω, equations (1-5) completely specify the boundary-value problem to be solved.

Approximate Solution for One-Dimensional Absorption

Consider the problem of infiltration from a saturated fracture at zero potential (located at $x=0$) into the adjacent semi-infinite formation ($x>0$). The assumption of a semi-infinite block should be valid for times small enough so that the wetting front has not reached the nearest other fracture. In this case, equations (1,4,5) take the form

$$\frac{\partial}{\partial x}\left[\beta k_r(\psi)\frac{\partial \psi}{\partial x}\right] = \frac{\partial S}{\partial t} \,, \tag{6}$$

$$\psi(x,0)=\psi_i \quad \text{for all } x>0 \,, \tag{7}$$

$$\psi(0,t)=0 \quad \text{for all } t>0 \,, \tag{8}$$

$$\lim_{x\to\infty}\psi(x,t)=\psi_i \quad \text{for all } t>0 \,. \tag{9}$$

The last condition (9) reflects the fact that at any finite time, the effect of the boundary condition at $x=0$ must become negligible as $x\to\infty$.

Because of the variation of k_r and S with ψ, equations (6-9) represent a highly nonlinear problem that is not amenable to standard analytical techniques such as Laplace transforms, Green's functions, etc. Nevertheless, much progress has been made in obtaining solutions to the absorption problem, for many different types of characteristic curves. Philip (1960) in fact derived a closed-form solution that requires the characteristic curves to be expressible as series of inverse error functions. Expressing (2) and (3) in this form, however, requires considerable computational effort, made particularly difficult by the relative obscurity of inverse error functions. 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 (Babu, 1976), iterative methods (Parlange, 1971), and variational principles (Parlange, 1975). Many of these methods are reviewed and discussed by Brutsaert (1976). 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 (1) and (2). They also have the disadvantage of not being extendable to geometries other than the half-space, since they rely on the similarity transformation $\eta = x/\sqrt{t}$.

A closed-form approximate solution can be obtained by using the so-called "boundary-layer", or "integral", technique. The boundary-layer method has been

widely used for heat conduction problems (Goodman, 1964), heat transfer problems with phase change (Eckert and Drake, 1972), and viscous flow problems (Schlichting, 1968). Prasad and Römkens (1982) used a related method to investigate vertical infiltration under time-varying boundary conditions. Although this method correctly predicts a similarity solution that depends on $x/\sqrt{t}$, it does not begin with this as an assumption, and therefore can be extended to geometries other than the half-space (Zimmerman and Bodvarsson, 1989), for which the similarity solution does not apply.

The integral method begins with the choice of a trial solution for the pressure or saturation profiles. 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 PDE, which is then integrated over the region Ω, the result is an ODE that describes the time evolution of δ. If a reasonable shape for the trial profile is assumed, the method is known to lead to accurate results for the types of problems mentioned above. The accuracy of the boundary-layer method for the present problem depends mainly on choosing an appropriate pressure profile. Although the potential, strictly speaking, does not reach ψ_i until $x \to \infty$, for practical purposes (Babu, 1976) it can be considered to equal ψ_i for all $x > \delta$, where δ is the penetration distance. As it turns out, it is convenient to use the saturation profile, rather than the potential profile, in the calculations. Hence we require that the trial profile satisfy the conditions $S(0,t) = S_s$, and $S(\delta,t) = S_i$.

The key to chosing a successful profile in this particular problem is having 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., $\psi(x,t) = -ax + \cdots$, 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 equation (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 $S(x,t) = S_s - bx^n + \cdots$, 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

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

$$S = S_i \quad \text{for } \delta < x < \infty . \tag{10}$$

It is often recommended (Goodman, 1964) that trial profiles should have zero slope at the edge of the boundary layer, so that the flux is continuous at $x = \delta$. While this condition is satisfied by the exact solution, since it merely reflects conservation of mass at the boundary between the disturbed and undisturbed zones, enforcing it would require a trial profile that contained an additional free parameter. This would substantially complicate the algebraic manipulations that are needed to solve the problem, without a concomitant increase in the accuracy of the results. It is simpler to imagine that there is a small tail on the saturation profile expressed by equation (10), providing continuity of flux at the outer edge of the boundary layer, but sufficiently localized so as to make no perceptible contribution to the mass conservation integral.

With the saturation profile given by equation (10), the conservation equation (6) is integrated from $x = 0$ to $x = \infty$. Using the facts that $\partial\psi/\partial x = 0$ for all $x > \delta$, and that $k_r = 1$ at $x = 0$, the left side of (6) can be integrated to yield

$$\int_0^\infty \frac{\partial}{\partial x}\left[\beta k_r(\psi)\frac{\partial\psi}{\partial x}\right] dx = -\beta\frac{\partial\psi}{\partial x}\bigg|_{x=0}$$

$$= \frac{\beta}{\alpha\delta}\left[\frac{(S_s - S_i)}{m(S_s - S_r)}\right]^{1/n} . \tag{11}$$

The right side of (6) integrates out to

$$\int_0^\infty \frac{\partial S}{\partial t} dx = \int_0^\delta n(S_s - S_i)(x/\delta)^n \frac{1}{\delta}\frac{d\delta}{dt} dx$$

$$= \int_0^1 n(S_s - S_i)\zeta^n \frac{d\delta}{dt} d\zeta = \frac{n(S_s - S_i)}{(n+1)} \frac{d\delta}{dt} . \tag{12}$$

Equating (11) and (12) leads to

$$\frac{\beta}{\alpha\delta}\left[\frac{(S_s - S_i)}{m(S_s - S_r)}\right]^{1/n} = \frac{n(S_s - S_i)}{(n+1)} \frac{d\delta}{dt} . \tag{13}$$

Since none of the parameters appearing in (13) vary with δ or t, and since $\delta = 0$ when $t = 0$, equation (13) can be integrated to yield

$$\delta = \left[\frac{2(n+1)kt}{\alpha n \mu\phi} \frac{(S_s - S_i)^{-1+1/n}}{[m(S_s - S_r)]^{1/n}}\right]^{1/2} . \tag{14}$$

Since δ grows as $\sqrt{t}$, and the saturation profile (10) is a function only of x/δ, the approximate solution has the self-similar structure that was shown by Bruce and Klute (1956) to hold regardless of the specific characteristic curves used.

The instantaneous volumetric flux at the wall is found by combining equations (11) and (14) with Darcy's law:

$$q = -\frac{kk_r}{\mu}\frac{\partial\psi}{\partial x}\bigg|_{x=0} = \frac{k}{\mu\alpha\delta}\left[\frac{(S_s - S_i)}{m(S_s - S_r)}\right]^{1/n}$$

$$= \left[\frac{nk\,\phi(S_s - S_i)^{1+1/n}}{2\alpha(n+1)\mu t\,[m\,(S_s - S_r)]^{1/n}}\right]^{1/2} . \tag{15}$$

The cumulative volumetric liquid flux is found by integrating equation (15) over time, which leads to

$$Q = \int_0^t q(\tau)\,d\tau = \left[\frac{2nk\,\phi t\,(S_s - S_i)^{1+1/n}}{\alpha\mu(n+1)[m\,(S_s - S_r)]^{1/n}}\right]^{1/2} . \tag{16}$$

Absorption from a Fracture in the Topopah Spring Formation

In order to determine the accuracy of the approximate solution, we can compare its predictions to the results of numerical simulations. The simulations were carried out using TOUGH (Pruess, 1987), an integrated-finite-difference program that is known to accurately model three-dimensional flow of water and air in porous media. The physical parameters used in these simulations are those that have been estimated for the Topopah Spring unit at Yucca Mountain. The Topopah Spring unit is a welded volcanic tuff with an estimated matrix permeability of 3.9×10^{-18} m^2, estimated 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 $\alpha = 1.147\times10^{-5}$ Pa^{-1} (Rulon et al., 1986).

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 estimated (Niemi and Bodvarsson, 1988) for the Topopah Spring

unit. These simulations, however, are intended mainly as a test of the approximate solutions, and not as predictions of actual processes at Yucca Mountain, for which more accurate physical property data would be needed. The viscosity of water was taken to be 1 cp, or 0.001 kg/ms. The block matrix was divided into 25 grid blocks, each 0.04 m thick. Sensitivity studies, as well as previous experience with TOUGH, have shown that for problems such as these, further refinement of the grid leads to improvements in accuracy on the order of only one percent.

Figure 4 shows the potential profile for this problem, after an elapsed time of 1×10^7s (116 days), according to both the approximate solution and the numerical simulation. Since the solution depends only on the similarity variable $\eta = x/\sqrt{t}$, the profiles would have the same shapes for any value of time. The saturation profile is shown in Figure 5. Since the instantaneous flux into the formation is proportional to the slope of the potential at the boundary, and 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. Note also that the approximate solution predicts the location of the wetting front with very high accuracy.

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. Martinez (1988) 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. The results showed that the precise details of the hydraulic properties of the fracture were relatively unimportant for this problem; the rate of advance of the front was influenced mainly by the

absolute permeability of the fracture.

We are interested in eventually solving large-scale problems using a numerical simulator such as TOUGH, with the approximate expression (15) serving as a source/sink term for the fracture elements. Use of this type of source/sink term will limit our 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 Figure 6, with the fracture oriented horizontally. Flow into the fracture is driven by the imposed potential at the $y=0$ boundary. For simplicity in this sample problem, we use the same characteristic curves as specified above for both the fracture and matrix, but a matrix permeability of 3.9×10^{-20} m^2, and a fracture permeability of 3.9×10^{-10} m^2. This fracture permeability corresponds roughly to an aperture of 100 μm, allowing for tortuosity and contact-area effects. The fracture is discretized into 10 elements, each 1 m long and 100 μm thick. Each of these elements has a "sink" term (for which TOUGH already has provisions), the magnitude of which varies with time according to equation (15). The sink is assumed to "turn on" instantaneously when the saturation in the block reaches 0.90, which is nominally considered 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 μm 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 Figure 7, 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 we are

modeling is not insignificant.

Conclusions

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. This solution has been compared to numerical simulations of this problem, using the hydraulic properties that have been estimated for the Topopah Spring welded tuff at Yucca Mountain, Nevada. The approximate solution was seen to predict both the infiltration rate and the location of the wetting front with high accuracy. 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. 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. Future work in this area will be aimed at generating source/sink approximations for finite-sized matrix blocks, and incorporating more realistic hydraulic properties for the fractures.

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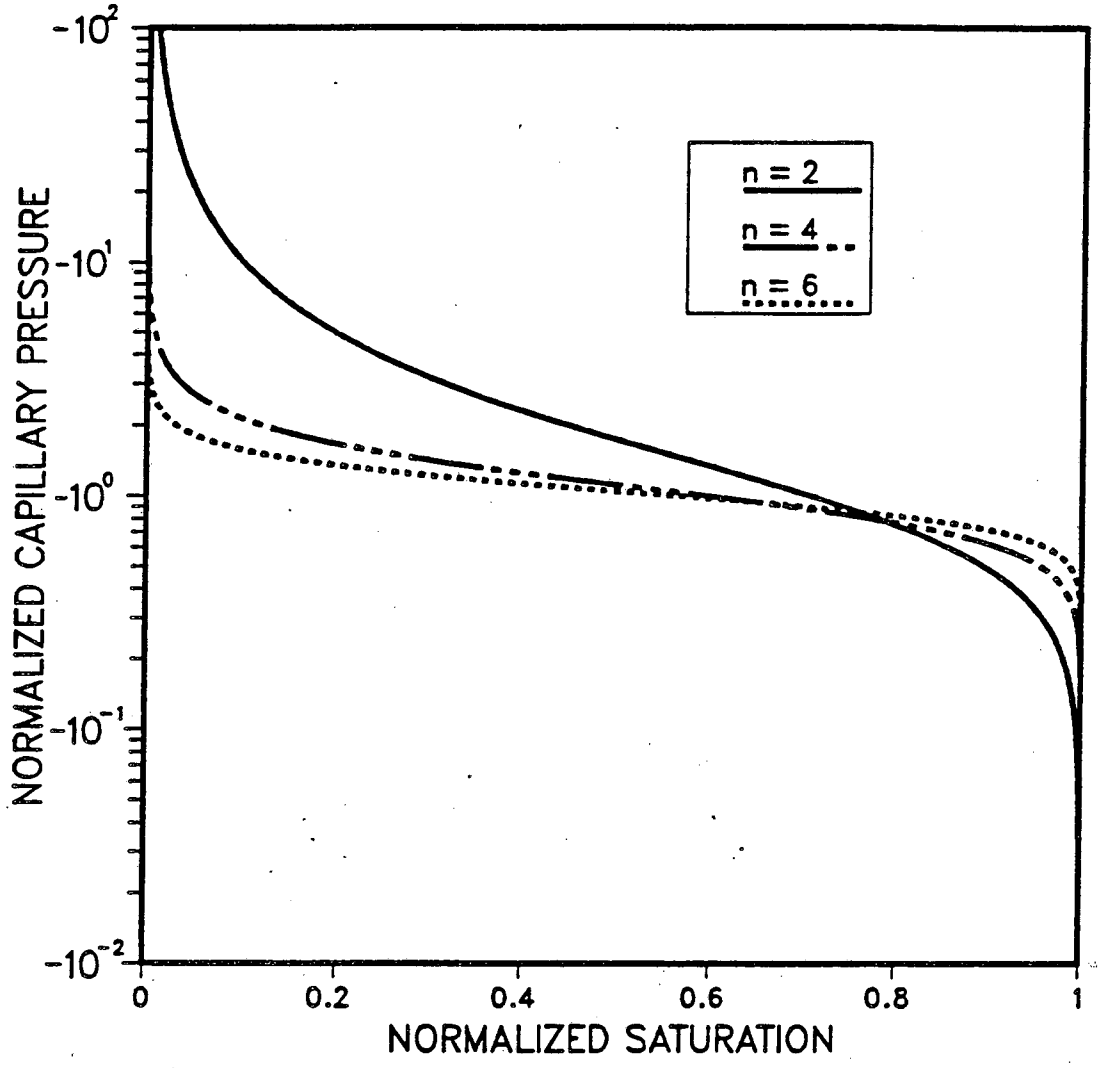

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Figure 1. Capillary pressure curves for a porous medium, according to the van Genuchten model. After normalization, the shapes of the curves depend only on the parameter n.

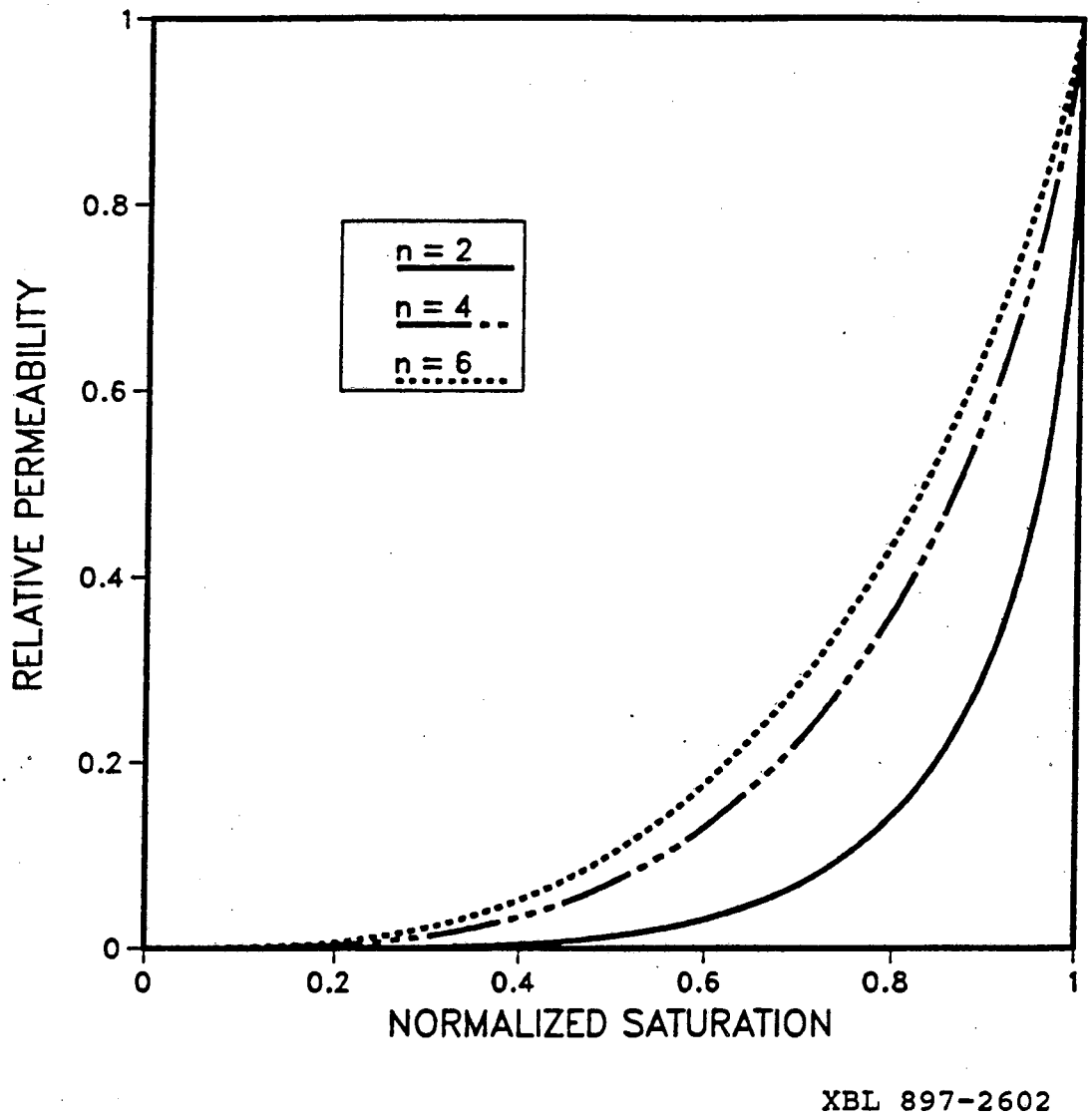

Figure 2. Relative permeability curves for a porous medium, according to the van Genuchten model. After normalization, the shapes of the curves depend only on the parameter n.

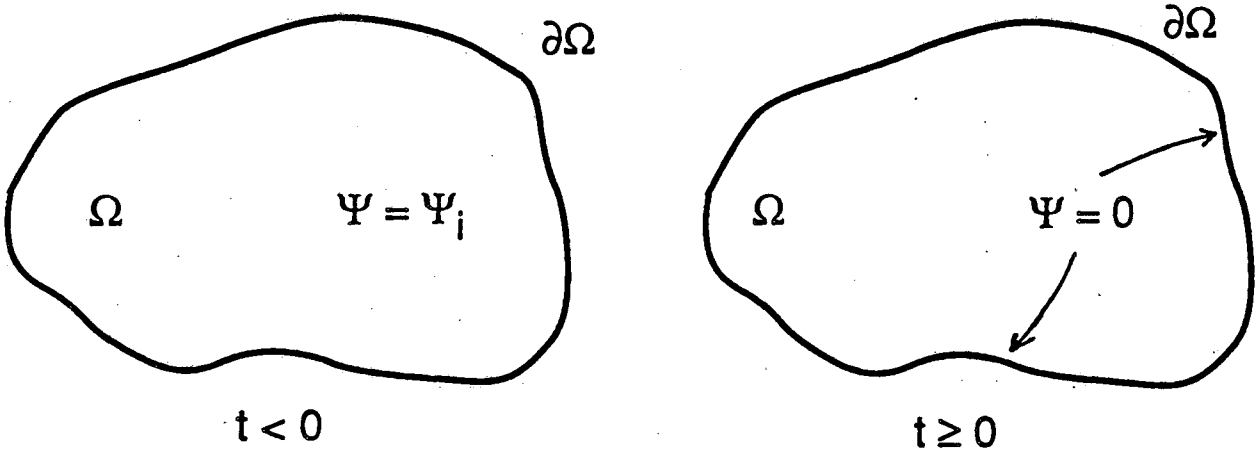

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Figure 3. Schematic diagram of the basic boundary-value problem of absorption into a porous block.

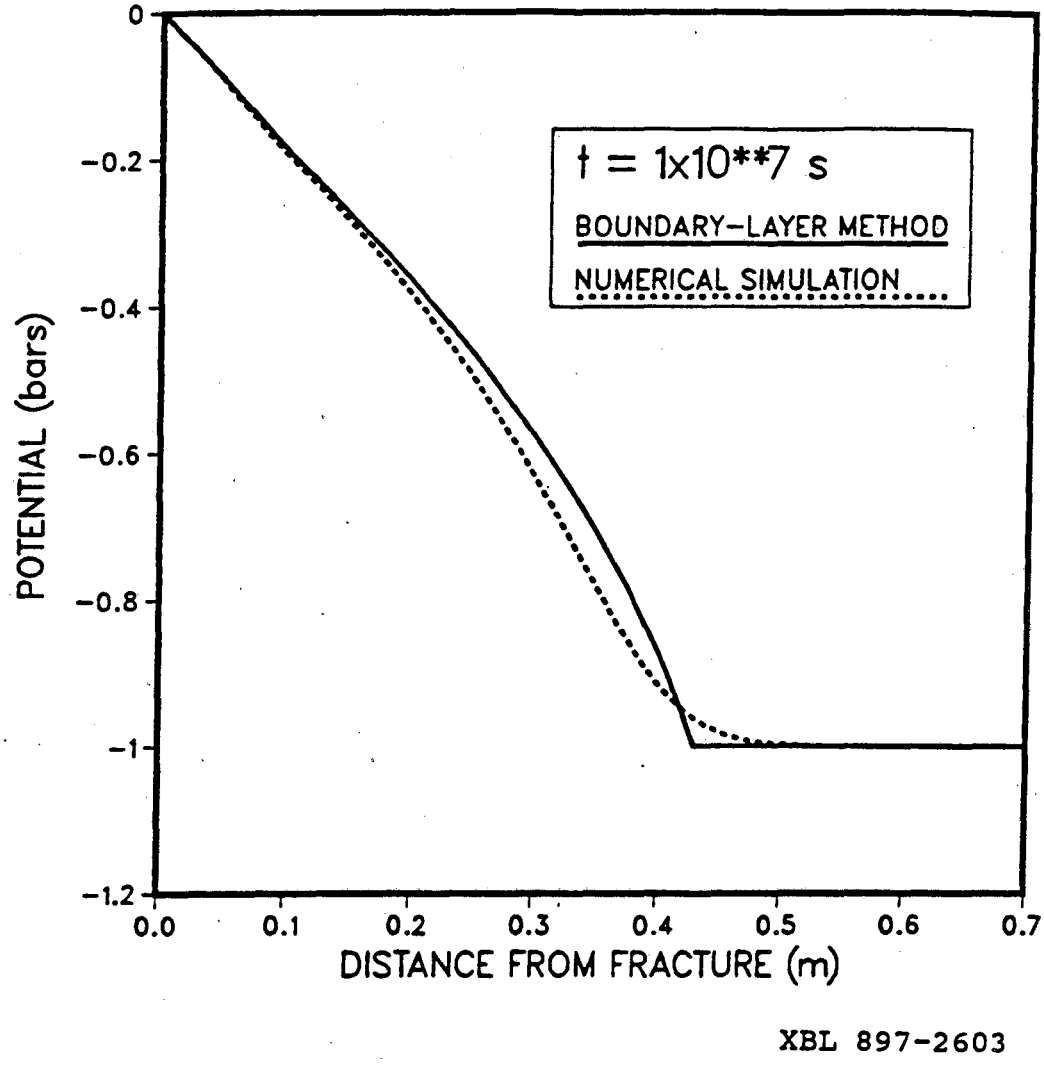

Figure 4. Potential profiles for one-dimensional absorption in Topopah Spring welded tuff. Physical properties of tuff are listed in text.

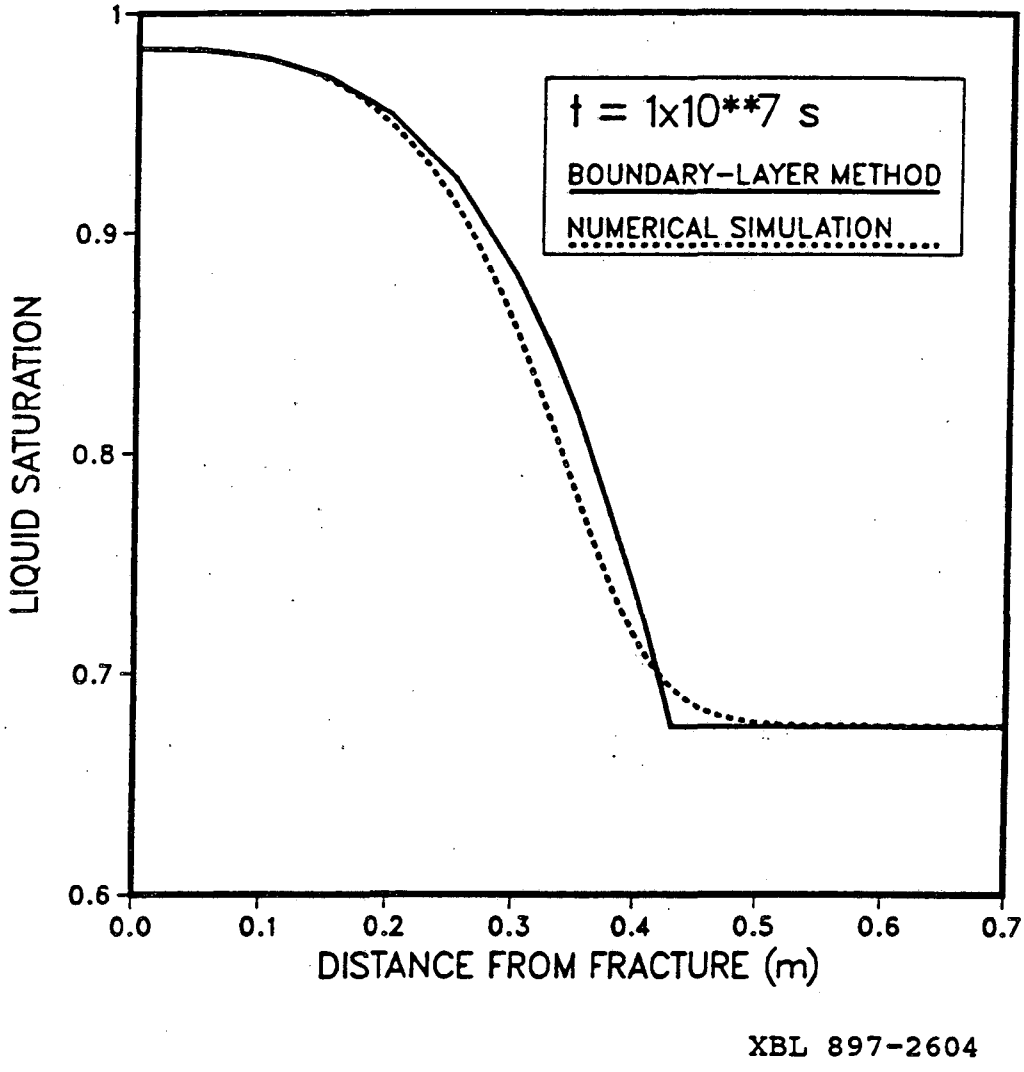

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Figure 5. Saturation profile for the same problem as shown in Figure 4.

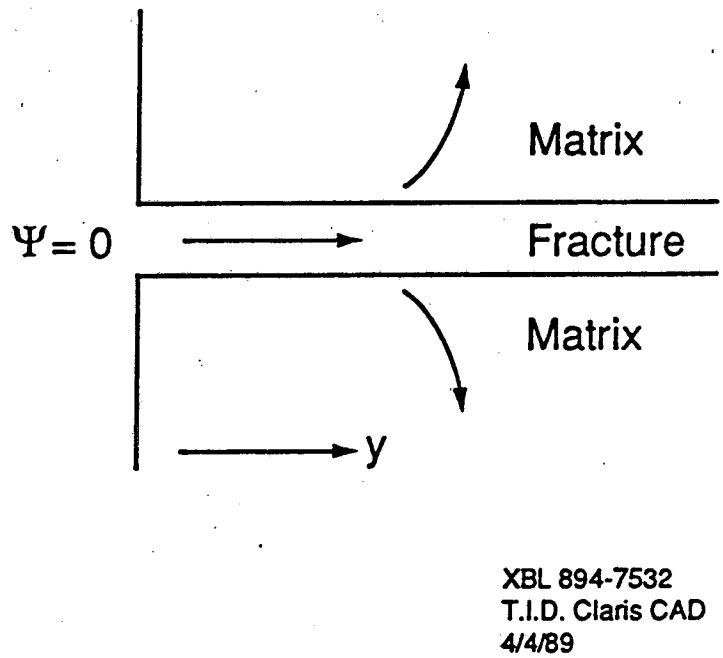

Figure 6. Schematic diagram of the problem of infiltration into a fracture, with transverse leakage into the matrix.

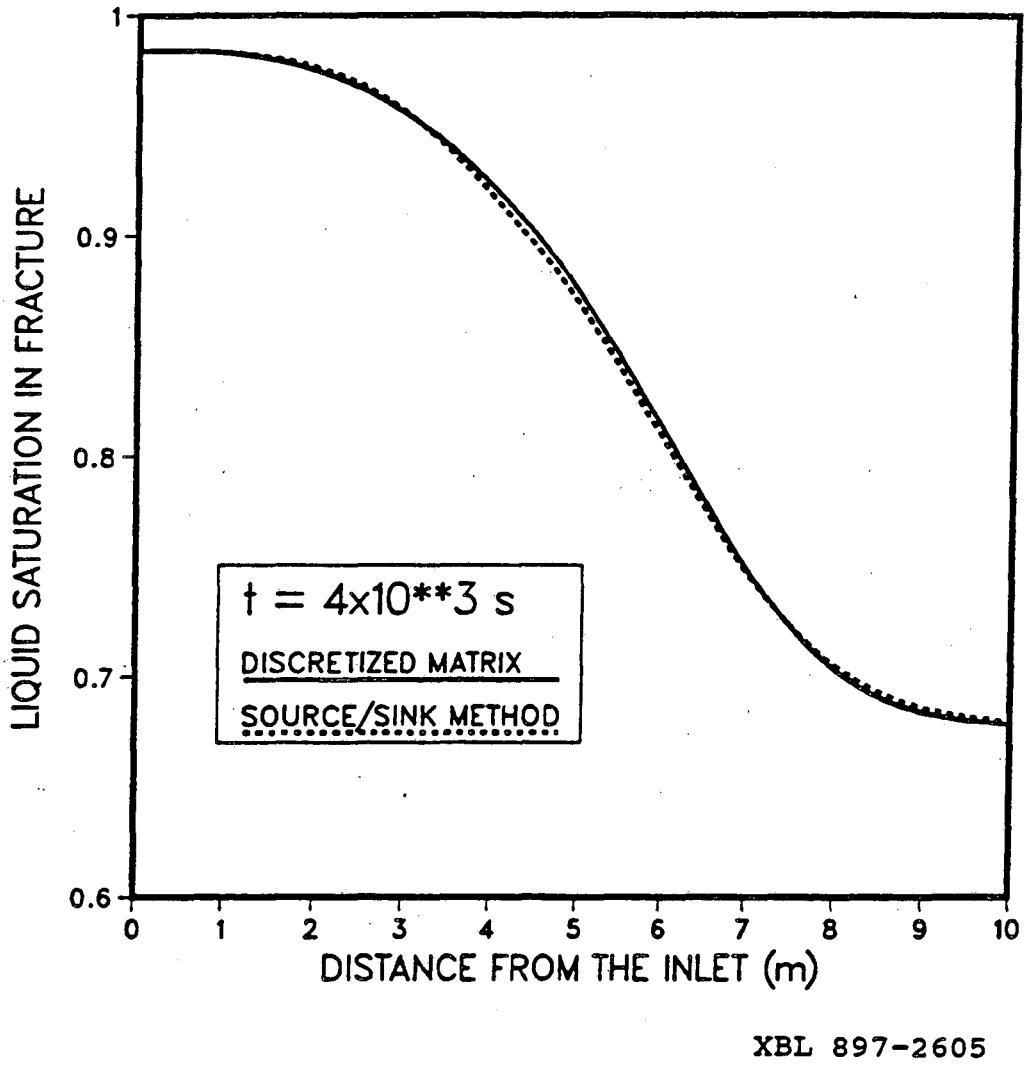

Figure 7. Saturation profile in fracture for flow along fracture with transverse leakage to matrix. Hydraulic properties used in simulations are listed in text.

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