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An Inverse Procedure for Estimating the Unsaturated Hydraulic Conductivities of Volcanic Tuffs

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Yucca Mountain, Nevada, is a potential site for a Department of Energy underground radioactive waste repository. The potential repository horizon is located above the water table in a formation consisting of volcanic tuffs. A key criterion in judging the suitability of the site is the rate, if any, at which precipitation percolates down to the water table. This flux of water could conceivably transport radionuclides to the saturated zone, so that they might eventually reach the groundwater supply. As water infiltrates down from the surface, it may at first flow mainly through the fracture network, but some of the water is imbibed from the fractures into the matrix blocks (Travis et al., 1984; Nitao and Buscheck, 1991). The rate at which this imbibition occurs is an important factor in determining whether water from a precipitation event is able to reach the water table or becomes absorbed into the matrix blocks and eventually evaporates out to the atmosphere. The parameters that determine this rate of matrix block imbibition include the size and shape of the matrix blocks, as well as the two characteristic functions of the tuff. These functions relate the water content of the tuff to its capillary pressure and its hydraulic conductivity. Because of the heterogeneity of the rocks at Yucca Mountain, it will be necessary to measure, or otherwise determine, these hydrologic properties at many locations. Because of the very small pore sizes of most of the tuffs found at Yucca Mountain, measurements of capillary pressure and hydraulic conductivity, as functions of water content, are very time-consuming, because these measurements require that either a steady state or an equilibrium state be reached. For this reason, it would be advantageous to be able to estimate the characteristic functions from other, more readily measurable properties.

One readily measurable property that is also of major importance to the overall hydrological behavior of Yucca Mountain is sorptivity (Philip, 1955), which quantifies the initial rate of imbibition during a one-dimensional imbibition process. The sorptivity is not a basic hydrological property of a rock, since it refers to a specific process. Nevertheless, it is related to, and is a function of, the above-mentioned characteristic functions. The advantage of measuring sorptivity is that because it intrinsically involves a transient process, measurements of sorptivity do not require that the sample reach equilibrium (or a steady state). We have developed an inverse procedure for using sorptivity measurements, along with measurements of the

capillary pressure function, to find the hydraulic conductivity function. This method has the advantage, unlike many other inversion procedures (cf. Mishra and Parker, 1989), of not restricting us *a priori* to any specific mathematical form for the characteristic functions. This allows us to derive characteristic curves that, when substituted into a numerical model of the unsaturated zone at Yucca Mountain (Wittwer et al., 1992), will yield computed sorptivities that agree exactly with the values measured in the laboratory. Such agreement is not possible in general if the characteristic functions are restricted in advance to be of a certain mathematical form.

SORPTIVITY OF UNSATURATED ROCK

The governing equation for one-dimensional flow of liquid water in an unsaturated porous medium is the Richards equation (Hillel, 1980):

$$\frac{\partial}{\partial x} \left[\frac{kk_r(\theta)}{\mu\phi} \frac{\partial \psi}{\partial x} \right] = \frac{\partial \theta}{\partial t} \quad (1a)$$

The parameter k , with dimensions of $[L^2]$, is the absolute permeability, which is the permeability of the medium when it is fully saturated with water. $k_r(\theta)$ is the dimensionless relative permeability function, which quantifies the extent to which partial saturation with air lowers the permeability of the liquid phase. μ is the viscosity of the water $[ML^{-1}T^{-1}]$, and ϕ is the porosity of the medium; in most treatments of absorption, both of these parameters are assumed to be constant. ψ is the capillary (matric) potential of the liquid in the porous medium, with dimensions of $[ML^{-1}T^{-2}]$, and θ is the degree of liquid saturation, which is defined as the water content divided by the porosity. The two functions $\psi(\theta)$ and $k_r(\theta)$ are often collectively referred to as the characteristic functions of the porous medium. In this form of the Richards equation, we ignore the gravitational term, since its effect is negligible during imbibition experiments conducted on small samples (Zimmerman et al., 1990).

Equation (1a) can be rewritten in a slightly different form that explicitly demonstrates that it is a nonlinear diffusion equation. Using the chain rule of differentiation gives

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$$\frac{\partial}{\partial x} \left[\frac{kk_r(\theta)}{\mu\phi} \frac{d\psi}{d\theta} \frac{\partial\theta}{\partial x} \right] \equiv \frac{\partial}{\partial x} \left[D(\theta) \frac{\partial\theta}{\partial x} \right] = \frac{\partial\theta}{\partial t}, \quad (1b)$$

in which the only independent variable that explicitly appears is θ . The diffusion coefficient $D(\theta)$ is given by $kk_r(\theta)\psi'(\theta)/\mu\phi$. The combination $kk_r\rho g/\mu$ is often referred to as the hydraulic conductivity, where ρ is the density of the fluid and g is the gravitational acceleration. Since ρ and μ are properties of the fluid, and not of the porous medium, we prefer to work with the combination $kk_r(\theta)$, which we will refer to as the permeability function of the medium.

The basic problem of one-dimensional absorption of water is specified by augmenting Eq. (1a) or (1b) with the following boundary/initial conditions:

$$\psi(x, t = 0) = \psi_i, \quad (2)$$

$$\psi(x = 0, t > 0) = \psi_w. \quad (3)$$

The values ψ_i and ψ_w can be related to saturations θ_i and θ_w through the capillary pressure function $\psi(\theta)$. A commonly used boundary condition is $\theta_w = 0$, which is usually assumed to correspond to full liquid saturation; i.e., $\theta_w = 1$. The solution to Eq. (1) for the boundary/initial conditions given by Eqs. (2) and (3) can be expressed in terms of the Boltzmann variable, $\eta = x/\sqrt{t}$ (see Hillel, 1980). This in turn implies that the cumulative influx into the medium, $I(t)$, which has dimensions of volume of liquid [L^3], will be proportional to the cross-sectional area A and also proportional to $t^{1/2}$. The constant of proportionality was called the "sorptivity" by Philip (1955), and denoted by S , so that

$$I(t) = SA t^{1/2}. \quad (4)$$

The sorptivity, which has dimensions of $[LT^{-1/2}]$, depends on the hydraulic properties of the porous medium, as well as on the initial saturation. If the hydraulic properties were known, the sorptivity could be found by solving the Richards equation using analytical or numerical methods. In practice, however, the sorptivity is much easier to measure than are either $\psi(\theta)$ or $kk_r(\theta)$. This suggests using measured values of the sorptivity to estimate the capillary pressure and/or permeability functions.

Two problems limit the possibility of finding a unique solution to estimating the characteristic functions from the sorptivity. First, since Eq. (1b) implies that $kk_r(\theta)$ and $\psi(\theta)$ affect S through the combination $kk_r(\theta)\psi'(\theta)$, it will not be possible to estimate $kk_r(\theta)$ and $\psi(\theta)$ separately. Furthermore, the sorptivity is generally not very sensitive to the diffusivity function. For example, the numerically computed sorptivity/saturation curves found by

Zimmerman and Bodvarsson (1989,1991a) for media with van Genuchten (1980) and Brooks and Corey (1966) characteristic functions can be made to closely coincide over large ranges of initial saturations by proper choice of the parameters (see Zimmerman et al., 1993). Hence it would be difficult to distinguish between these two types of characteristic functions on the basis of their measured sorptivities.

INVERSION PROCEDURE

One feature of the sorptivity-saturation relationship that follows from both the van Genuchten and Brooks-Corey characteristic functions is that the $S(\theta_i)$ curve is concave downward and typically has a very steep (actually, infinite) slope at $\theta_i = 1$. In particular, for initial saturations that are close to 1, the sorptivity of a Brooks-Corey medium is proportional to $(1 - \theta_i)^{1/2}$ (Zimmerman and Bodvarsson, 1991a), whereas the sorptivity of van Genuchten media varies as $(1 - \theta_i)^{(n+1)/2n}$, where $n > 2$ is the van Genuchten parameter (Zimmerman and Bodvarsson, 1991b). No admissible choice of the van Genuchten or Brooks-Corey parameters will lead to sorptivities that are linear functions of the initial saturation. Some measured sorptivities of volcanic tuffs from Yucca Mountain, Nevada (Flint et al., 1993), however, have been found to be fairly well fitted with functions of the form $S(\theta_i) = S_{\max}(1 - \theta_i)$, where S_{\max} is a fitting parameter. To model these samples, we cannot use Brooks-Corey or van Genuchten characteristic functions but must find characteristic functions that lead to linear sorptivities.

To carry out our inversion procedure, we first note (Warrick and Broadbridge, 1992) that if the hydraulic diffusivity function $D(\theta)$ is a constant, say D_0 , the sorptivity will have the form $S(\theta_i) = 2\phi\sqrt{D_0/\pi}(1 - \theta_i)$. A constant diffusivity is therefore consistent with the result $S = S_{\max}(1 - \theta_i)$ if we make the identification

$$D_0 = \frac{\pi S_{\max}^2}{4\phi^2}. \quad (5)$$

Some evidence that a linear sorptivity-saturation relationship corresponds *uniquely* to a constant hydraulic diffusivity is given by Zimmerman et al. (1993). Assuming therefore that the diffusivity is constant, the following relationship holds between $kk_r(\theta)$ and $\psi(\theta)$:

$$kk_r(\theta) = \frac{\mu\phi D_0}{\psi'(\theta)}, \quad (6)$$

which can be combined with Eq. (5) to yield

$$kk_r(\theta) = \frac{\pi\mu S_{\max}^2}{4\phi\psi'(\theta)} \quad (7)$$

If we can determine S_{\max} and $\psi(\theta)$ experimentally, Eq. (7) can then be used to predict the hydraulic permeability. Testing this method would require measurements of all three functions, $S(\theta_i)$, $kk_r(\theta)$, and $\psi(\theta)$. Currently, reliable data for all three of these functions are not available for many samples. As an example and test case for the method, consider sample 1UH, which is a vitrified tuff from the Calico Hills unit, with a porosity ϕ of about 0.39 (Flint and Flint, 1990). Figure 1 shows three measured values of the sorptivity as a function of initial saturation, which have been fitted with a curve of the form $S(\theta_i) = S_{\max}(1 - \theta_i)$. The value of S_{\max} was found to be $9.44 \times 10^{-5} \text{ m}^2/\text{s}$. Figure 2 shows the measured capillary pressures for this sample, fitted to a curve of the form $\psi(\theta) = \psi_a\theta^{-m}$, with $\psi_a = -1.50 \times 10^4 \text{ Pa}$ and $m = 5.45$. Since $\psi'(\theta) = -m\psi_a\theta^{-(m+1)}$, Eq. (7) yields

$$kk_r(\theta) = \frac{\pi\mu S_{\max}^2 \theta^{m+1}}{4\phi(-m)\psi_a} = 2.19 \times 10^{-16} \theta^{6.45} \text{ m}^2, \quad (8)$$

in which the viscosity of water is taken to be 0.001 Pa·s. Figure 3 shows the permeabilities that were measured by Flint and Flint (1990) using the centrifuge method, along with those predicted by Eq. (8). The agreement is seen to

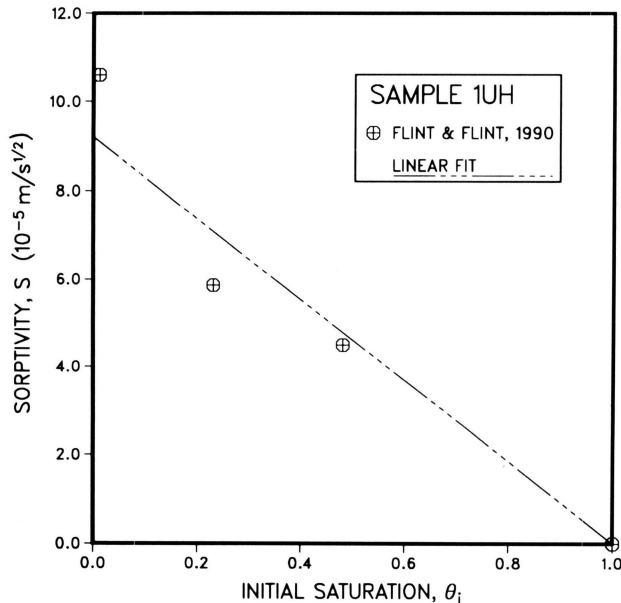


Figure 1. Sorptivity of sample 1UH, a vitrified tuff from the Calico Hills unit at Yucca Mountain, at several different initial saturations. The straight line was found by a least-squares fit to the function $S(\theta_i) = S_{\max}(1 - \theta_i)$. S_{\max} was found to be $9.44 \times 10^{-5} \text{ m}^2/\text{s}^{1/2}$. [XBL 936-881]

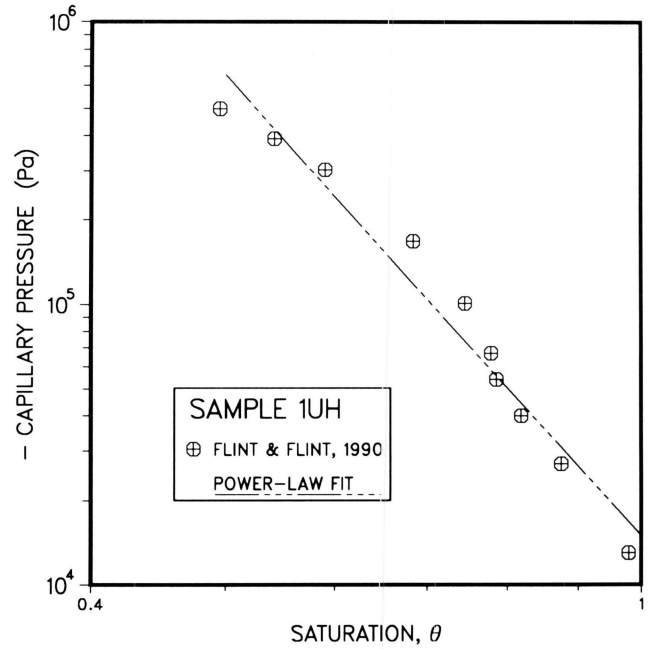


Figure 2. Capillary pressure of sample 1UH. The straight line was found by fitting $\psi(\theta)$ to a curve of the form $\psi = \psi_a\theta^{-m}$. The fitting parameters were found to be $\psi_a = -1.497 \times 10^4 \text{ Pa}$ and $m = 5.45$. [XBL 936-882]

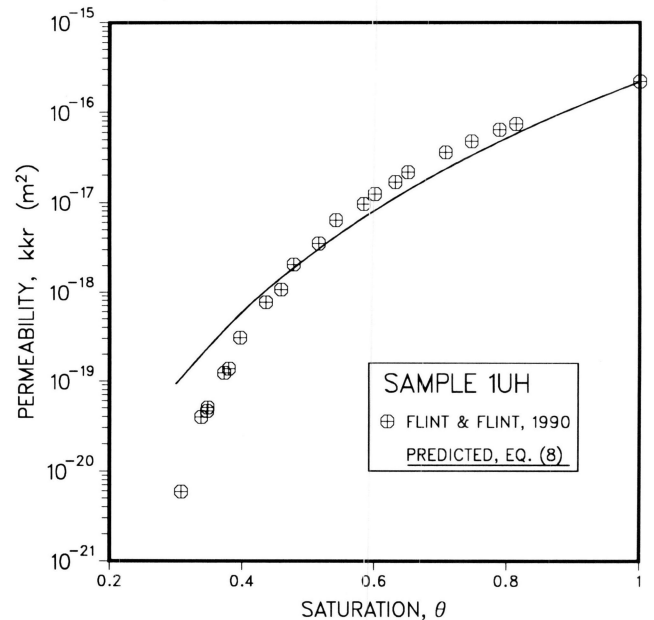


Figure 3. Hydraulic permeability of sample 1UH, as a function of saturation. The measured values are compared to the curve predicted by the inversion procedure: $kk_r(\theta) = 2.19 \times 10^{-16} \theta^{6.45} \text{ m}^2$. [XBL 936-883]

be fairly close, particularly when the saturation is greater than 0.40. For lower saturations, the curve in Figure 3 represents an extrapolation outside of the range where $\psi(\theta)$ data exist (see Figure 2).

SUMMARY AND CONCLUSIONS

Measurements made by Flint et al. (1993) showed that the sorptivities of some volcanic tuffs from Yucca Mountain were linear functions of the initial saturation. This is consistent with the hydraulic diffusivities of these tuffs being constant functions of the saturation. The assumption of constant diffusivity then leads to a one-to-one relationship between the capillary pressure function and the hydraulic permeability. Hence, we can use measurements of the sorptivity and capillary pressure, as functions of saturation, to find the permeability function. As an illustration of the inversion procedure, we applied this procedure to measurements on a sample of a vitrified tuff from the Calico Hills unit. The predicted permeability function was in reasonable agreement with the measured values. More data are needed to determine if this method can be reliably used to routinely predict permeabilities from the more readily measurable properties of sorptivity and capillary pressure.

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