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and L.E. Flint

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**An Inverse Procedure for Estimating
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AN INVERSE PROCEDURE FOR ESTIMATING
THE UNSATURATED HYDRAULIC CONDUCTIVITIES OF VOLCANIC TUFFS

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ABSTRACT

A procedure is developed for estimating the hydraulic conductivity function of unsaturated volcanic tuff, using measurements of the sorptivity and capillary pressure functions. The method assumes that the sorptivity is a linear function of the initial saturation, as is suggested by experimental data. The procedure is tested on a vitrified tuff from the Calico Hills unit at Yucca Mountain, and the predicted conductivities are in reasonable agreement with measured values. Further tests of this method are needed to establish whether or not it can be routinely used for conductivity predictions.

INTRODUCTION

Yucca Mountain, Nevada, is a potential site for a U. S. 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. As this occurs, some of the water is imbibed from the fractures into the matrix blocks.^{1,2} The rate at which this imbibition occurs is an important factor in determining whether or not water from a precipitation event is able to reach the water table, or whether it is absorbed into the matrix blocks and eventually evaporates out to the atmosphere. (Other methods are also being used to determine whether or not surface water has been able in the past to percolate down to the water table; these include hydrochemical studies and nuclear logging techniques). 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 found at Yucca Mountain, it will be necessary to measure, or otherwise determine, these hydrologic properties at many locations. Due to 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 either a steady state (or an equilibrium state) to 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, which quantifies the initial rate of imbibition during a one-dimensional imbibition process without gravity.³ 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, its measurement does not require the attainment of equilibrium (or a steady-state). We have developed an inverse procedure for using sorptivity measurements, along with measurements of one of the two characteristic functions, to find the other characteristic function. This method has the advantage, unlike many other inversion procedures, of not restricting us *a priori* to any specific mathematical form for the characteristic functions.^{4,5} This allows us to derive characteristic curves which, when substituted into a numerical model of the unsaturated zone at Yucca Mountain,⁶ will yield computed sorptivities that agree exactly with the values measured in the laboratory. Such agreement is not in general possible 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 a partially saturated (also called "unsaturated") porous medium is the Richards equation:⁷

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

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 have ignored the gravitational term, since its effect is negligible during imbibition experiments conducted on small samples.^{8,9}

Equation (1a) is sometimes rewritten in a form that explicitly demonstrates that it is a nonlinear diffusion equation.¹⁰ Using the chain rule of differentiation, we have

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

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 $\psi_w=0$, which is usually assumed to correspond to full liquid saturation, i.e., $\theta_w=1$. The problem posed by eqs. (1)-(3) is the basic problem of unsaturated flow. It applies to one-dimensional horizontal absorption, as well as to the early stages of vertical infiltration,¹¹ and the early stages of two- or three-dimensional infiltration problems.^{11,12}

SORPTIVITY-SATURATION RELATION

Since the Richards equation (1b) is a diffusion equation, its solution for the boundary/initial conditions given by eqs. (2,3) can be expressed in terms of the Boltzmann variable,⁷ $\eta = x/\sqrt{t}$. This in turn implies¹³ 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 $t^{1/2}$. This latter fact is true regardless of the specific forms of the characteristic functions. The constant of proportionality is called the "sorptivity" and is denoted by S , so that³

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

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. The sorptivity can be found (exactly) by solving the Richards equation using analytical or numerical methods,^{14,15} or from various sorptivity approximations that have been proposed.^{10,16} These approximations typically give the sorptivity in terms of certain integrals of the hydraulic diffusivity, and do not require solution of the governing differential equation. The sorptivity depends on the capillary pressure and permeability, which are more basic constitutive functions, whereas the sorptivity itself is process-dependent. However, it has often been pointed out that in practice the sorptivity is much easier to measure than are either $\psi(\theta)$ or $kk_r(\theta)$.¹⁴ This suggests using measured values of the sorptivity to estimate the capillary pressure and/or permeability functions. Specifically, if one has measured values of the sorptivity over the entire range of initial saturations, the question is raised as to what can be inferred about $\psi(\theta)$ and $kk_r(\theta)$.

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, in the sense that plots of sorptivity vs. initial saturation can often be very similar, for quite different sets of characteristic functions. For example, the numerically computed sorptivity/saturation curves found by Zimmerman and Bodvarsson^{15,17} for media with van Genuchten¹⁸ and Brooks-Corey¹⁹ characteristic functions can be made to closely coincide over large ranges of initial saturations by proper choice of the parameters. For example, consider the sorptivities plotted in Fig. 1, which were computed numerically using Brooks-Corey and van Genuchten functions. If the van Genuchten α parameter is chosen to be the reciprocal of the Brooks-Corey air-entry pressure, then the sorptivities can be directly compared in normalized form. In this example, the van Genuchten n parameter was taken to be 3. In order to make the two capillary pressure curves agree asymptotically at low saturations,²⁰ the Brooks-Corey λ parameter was taken to be 2 (i.e., $\lambda=n-1$). Fig. 1 shows that the two computed sorptivity curves agree very closely. Despite this, Brooks-Corey and van Genuchten soils have qualitatively different capillary pressure functions, since the van Genuchten model exhibits a smooth variation of ψ with θ , whereas in the Brooks-Corey model ψ is not a single-valued function of θ . Nevertheless, these two very different types of capillary pressure functions would be difficult to distinguish on the basis of their associated sorptivities.

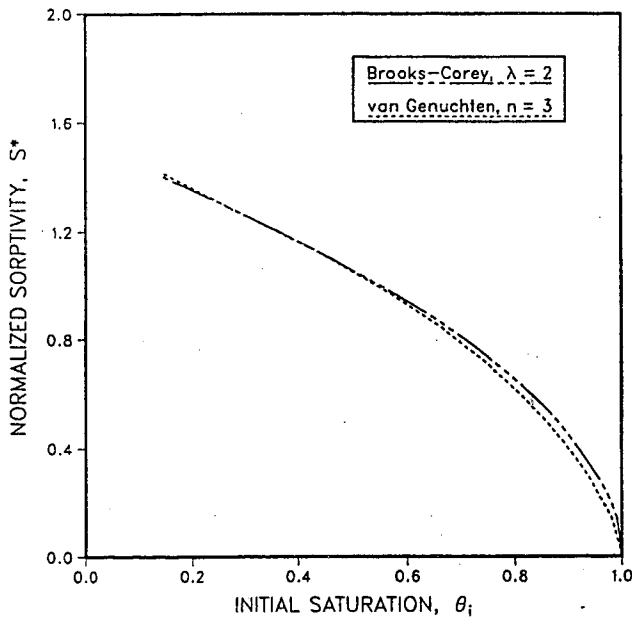


Fig. 1. Normalized sorptivities $S^* = S\sqrt{\alpha\mu/k\phi}$, computed using Brooks-Corey and van Genuchten characteristic curves. The two curves differ significantly only in the region of high initial saturations.

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 $\theta_i = 1$. This is demonstrated in the numerical results shown in Fig. 1, and also can be corroborated by use of approximate methods that exist for estimating the sorptivity directly from $D(\theta)$. In particular, for initial saturations that are close to 1, the sorptivity of a Brooks-Corey medium is proportional to $(1 - \theta_i)^{1/2}$, whereas the sorptivity of a van Genuchten media varies as $(1 - \theta_i)^{(n+1)/2n}$, where n is the van Genuchten parameter.^{17,21} Since the parameter n is restricted²² to the range $n > 2$, no choice of the van Genuchten parameter n will lead to sorptivities that are linear functions of the initial saturation. Some measured sorptivities of volcanic tuffs from Yucca Mountain, Nevada have, however, been found to be nearly linear functions of θ_i .²³ These sorptivities cannot be fit to van Genuchten or Brooks-Corey characteristic curves, by any allowable choice of the open parameters. Hence, in order to model these samples, we must find characteristic functions that lead to linear sorptivities.

LINEAR SORPTIVITY FUNCTIONS $S(\theta_i)$

The experimental method used to measure sorptivity, which is described in detail by Flint et al.,²³ can be summarized as follows. A cylindrical rock core with a known initial saturation θ_i is placed atop a fritted glass disk, which sits inside an inverted funnel (see Fig. 2). The core and funnel are surrounded with a barrier to prevent loss of moisture. Tubing connects the bottom of the funnel to a water-filled

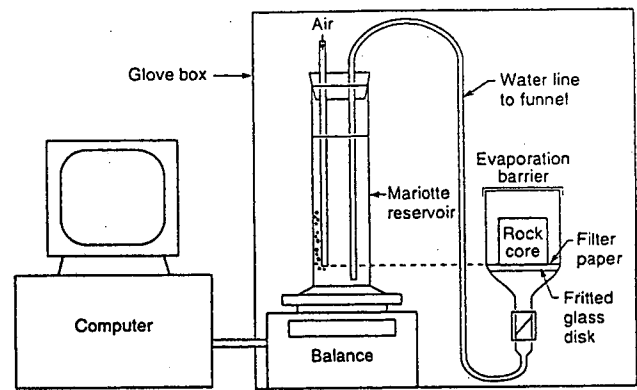


Fig. 2. Schematic diagram of the apparatus used to measure sorptivity (after Flint et al.²³). The fluid imbibed by the core is measured by monitoring the weight of the reservoir.

Mariotte reservoir. The reservoir is placed on an automated balance, and its weight is continuously recorded by a computer. The amount of liquid lost by the reservoir is assumed to be equal to that imbibed by the core, which (after conversion from weight to volume) yields the cumulative imbibition $I(t)$. The sorptivity $S(\theta_i)$ is found from eq. (4), by plotting $I(t)/A$ vs. $t^{1/2}$, and finding the slope of the resulting straight line.

The measurements of Flint et al.²³ indicate that the sorptivities of many volcanic tuffs can be fit to a function of the form $S(\theta_i) = S_{\max}(1 - \theta_i)$, where S_{\max} is a fitting parameter. Fig. 3 shows the measured sorptivities for a suite of samples that included nonwelded zeolitized tuffs, nonwelded silicified tuffs, and welded tuffs. Most can be reasonably well-fit by a straight line through the point $(S=0, \theta_i=1)$. To carry out our inversion procedure, we first note that if the hydraulic diffusivity $D(\theta)$ is a constant, say D_0 , the sorptivity will have the form $S = 2\phi\sqrt{D_0}\pi(1 - \theta_i)$.²⁴ A constant diffusivity is therefore consistent with the result $S = S_{\max}(1 - \theta_i)$. The next question is whether or not $D(\theta) = D_0$ is the *only* diffusivity function that leads to a linear sorptivity/saturation relationship. Although we have not been able to prove this, there is some evidence that it is the case. First, consider the sorptivity approximation suggested by Philip, which can be written as¹¹

$$S^2(\theta_i) = \frac{8\phi^2}{\pi} \int_{\theta_i}^1 (\theta - \theta_i) D(\theta) d\theta. \quad (5)$$

Now consider eq. (5) with $S(\theta_i) = S_{\max}(1 - \theta_i)$:

$$S_{\max}^2(1 - \theta_i)^2 = \frac{8\phi^2}{\pi} \int_{\theta_i}^1 (\theta - \theta_i) D(\theta) d\theta. \quad (6)$$

Differentiation of both sides of eq. (6) with respect to θ_i , using Leibnitz' rule to account for the appearance of θ_i both inside the integral and as one of the endpoints, yields

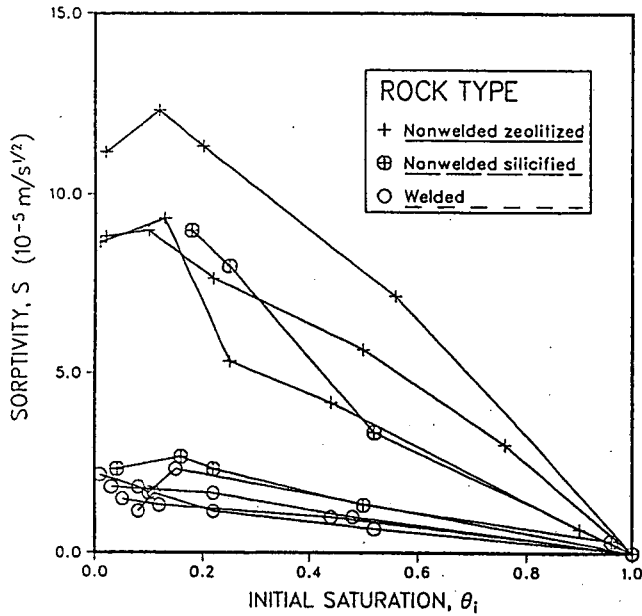


Fig. 3. Measured sorptivities of a suite of volcanic tuffs, as functions of the initial saturation.²³ Many of the samples exhibit a linear relationship between S and θ_i .

$$-2S_{\max}^2(1-\theta_i) = -\frac{8\phi^2}{\pi} \int_{\theta_i}^1 D(\theta) d\theta, \quad (7)$$

where we make use of the fact that the integrand goes to zero at the lower endpoint $\theta = \theta_i$. Another differentiation with respect to θ_i yields

$$2S_{\max}^2 = \frac{8\phi^2}{\pi} D(\theta_i), \quad (8a)$$

which can be solved to yield

$$D(\theta_i) = \frac{\pi S_{\max}^2}{4\phi^2}. \quad (8b)$$

Since θ_i is arbitrary in eq. (8b), this implies that $D(\theta) = D_0 =$ constant for all θ . Hence, at least according to Philip's sorptivity approximation, a diffusivity of the form $S(\theta_i) = S_{\max}(1-\theta_i)$, corresponds *uniquely* to a constant diffusivity D_0 , with $S_{\max} = 2\phi\sqrt{D_0/\pi}$.

Further indirect evidence that a linear sorptivity can correspond only to a constant diffusivity can be found in the numerical solutions computed by Kutilek and Valentová for the family of diffusivities of the form $D(\theta) = D_0 \exp(\beta\theta)$, where β is some constant parameter that characterizes each soil.¹⁶ They found that the $S(\theta_i)$ curve is concave up for $\beta < 0$, concave down for $\beta > 0$, and linear only when $\beta = 0$, i.e., for

$D(\theta) = D_0$. In light of the above facts, we make the assumption that a linear sorptivity function implies that $D(\theta)$ is constant. From the definition of the diffusivity in eq. (1b), we have (in general)

$$D(\theta) = \frac{kk_r(\theta) d\psi(\theta)}{\mu\phi d\theta}. \quad (9)$$

If $D(\theta) = D_0$, then we can solve eq. (9) to find, say, the capillary pressure function $\psi(\theta)$ in terms of the permeability function $kk_r(\theta)$. First, we solve for $d\psi/d\theta$:

$$\frac{d\psi(\theta)}{d\theta} = \frac{\mu\phi D_0}{kk_r(\theta)}. \quad (10)$$

We now integrate eq. (10), using the condition that $\psi = 0$ when $\theta = 1$, to find

$$\psi(\theta_i) = \mu\phi D_0 \int_{\theta_i}^1 \frac{d\theta}{kk_r(\theta)}. \quad (11)$$

Alternatively, we can solve eq. (9) for the hydraulic permeability, $kk_r(\theta)$, in terms of $\psi(\theta)$, which leads to

$$kk_r(\theta) = \frac{\mu\phi D_0}{d\psi/d\theta}. \quad (12)$$

Eqs. (11) and (12) allow one of the characteristic functions to be determined from knowledge of the other, if the sorptivity is of the form $S = S_{\max}(1-\theta_i)$.

INVERSION OF EXPERIMENTAL SORPTIVITIES

Consider the sorptivities measured by Flint et al. on a suite of volcanic tuffs from Yucca Mountain.²³ As mentioned above, these rocks exhibited nearly linear relationships between sorptivity and initial saturation, and therefore cannot be made to correspond to van Genuchten or Brooks-Corey characteristic curves, by any choices of the parameters. For rocks with a linear $S(\theta_i)$ relationship, eqs. (11) and (12) allow the calculation of one of the characteristic functions in terms of the other. Since it was found by Flint and Flint that the hydraulic permeability $kk_r(\theta)$ is the more difficult property to measure,²⁵ we will attempt to predict $kk_r(\theta)$ from measurements of $S(\theta_i)$ and $\psi(\theta)$. First, we fit the sorptivities to a function of the form $S(\theta_i) = S_{\max}(1-\theta_i)$, to find the fitting parameter S_{\max} . The diffusivity D_0 is then found from eq. (8) to be $D_0 = \pi S_{\max}^2 / 4\phi^2$. We then fit the capillary pressure data with any convenient type of function, and use eq. (12) to predict the permeability function.

Testing of this method requires 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

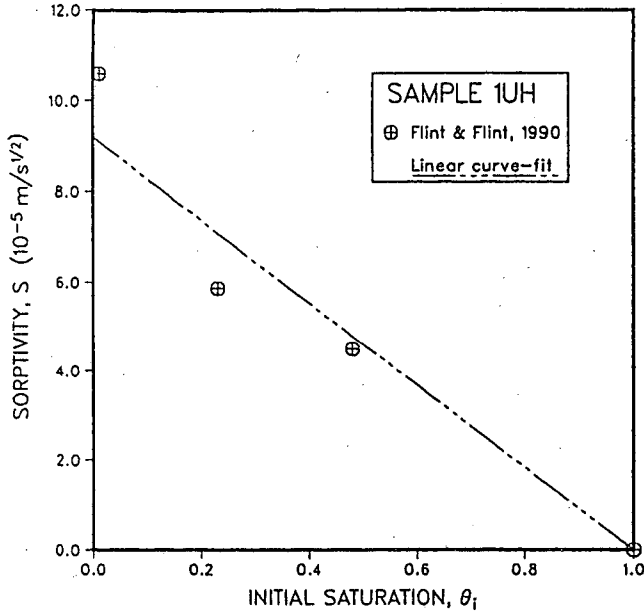


Fig. 4. Sorptivity of sample 1UH, a vitrified tuff from the Calico Hills unit at Yucca Mountain, at several different initial saturations. The straight line was found by a least-squares fit to the function $S(\theta_i) = S_{\max}(1 - \theta_i)$. S_{\max} was found to be $9.44 \times 10^{-5} \text{ m/s}^{1/2}$.

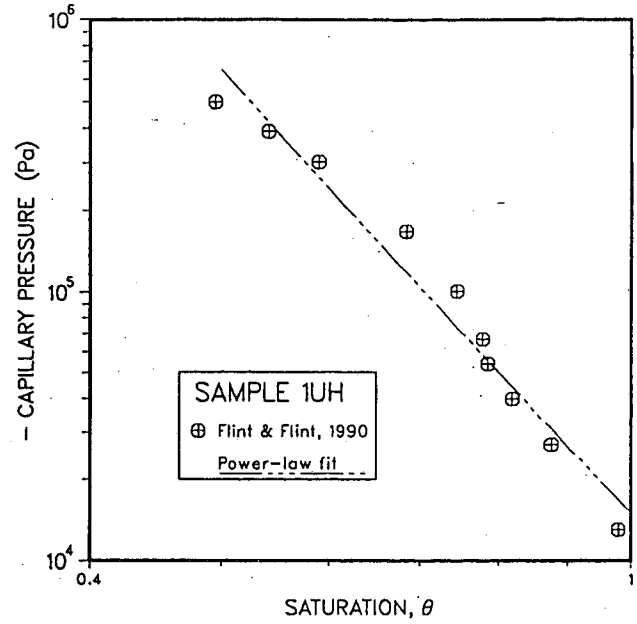


Fig. 5. Capillary pressure of sample 1UH (see Fig. 4). The straight line was found by fitting $\psi(\theta)$ to a curve of the form $\psi = \psi_a \theta^{-m}$. The fitting parameters were found to be $\psi_a = -1.497 \times 10^4 \text{ Pa}$, and $m = 5.45$.

a porosity ϕ of about 0.39.²⁵ Fig. 4 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 $9.44 \times 10^{-5} \text{ m}^2/\text{s}$. Fig. 5 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 $m = 5.45$. We now combine eqs. (8) and (12) to find

$$\begin{aligned} k k_r(\theta) &= \frac{\pi \mu S_{\max}^2}{4\phi(d\psi/d\theta)} = \frac{\pi \mu S_{\max}^2 \theta^{m+1}}{4\phi(-m)\psi_a} \\ &= 2.19 \times 10^{-16} \theta^{6.45} \text{ m}^2, \end{aligned} \quad (13)$$

in which the viscosity of water is taken to be 0.001 Pa·s, and $d\psi/d\theta = -m\psi_a \theta^{-(m+1)}$. Fig. 6 shows the permeabilities that were measured by Flint and Flint using the centrifuge method,²⁵ along with those predicted by eq. (13). The agreement is seen to be fairly close, particularly when the saturation is not less than 0.40. The permeability prediction was based on a capillary pressure curve which itself was derived from measurements for saturations above 0.495. In this range, the predicted permeabilities are always within a factor of two of the measured values, despite the fact that the permeability varies by three orders of magnitude. For lower saturations, the curve in Fig. 6 represents an extrapolation outside of the range where $\psi(\theta)$ data exist, and is less accurate.

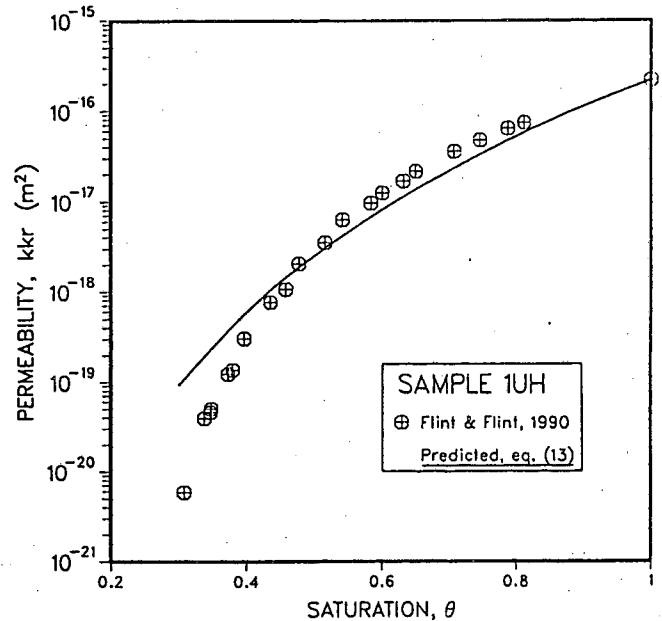


Fig. 6. Hydraulic permeability of sample 1UH (see Figs. 4,5), as a function of saturation. The measured values are compared to the curve predicted by the inversion procedure: $k k_r(\theta) = 2.19 \times 10^{-16} \theta^{6.45} \text{ m}^2$.

SUMMARY AND CONCLUSIONS

Measurements made by Flint et al. showed that the sorptivity of some volcanic tuffs from Yucca Mountain were linear functions of the initial saturation.²³ We have presented some evidence that this implies that the hydraulic diffusivity $D(\theta)$ is constant. 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.

As part of the process of characterizing the suitability of Yucca Mountain as a potential location of an underground radioactive waste repository, a detailed numerical model is being constructed to study the unsaturated zone hydrology.⁶ In order for the model to be as realistic as possible, accurate hydrological data are needed for the various geologic strata. The numerical model requires capillary pressure and permeability curves for each rock type. The sorptivity is not explicitly required as an input, since sorptivity is a process-dependent property, and not a fundamental constitutive parameter. Nevertheless, the sorptivity is an extremely important hydrologic property of the tuffs, since absorption of liquid from the fractures into the matrix blocks is the key process that will control the ability of (possibly radioactive) water to reach the water table, from which it may enter the groundwater system.^{2,26} As mentioned above, it is very difficult and time-consuming to make accurate measurements of the hydraulic permeability of a rock having such small pores. Sorptivity measurements, on the other hand, can be made relatively quickly and accurately. The procedure we have outlined above, if shown to be reliable and accurate, has the potential to allow the prediction of permeabilities. The method also has the advantage of assuring that the characteristic curves used as input to numerical models lead to the correct sorptivity.

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