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Abstract

The hydraulic conductivity functions of the matrix rocks at Yucca Mountain, Nevada, are among the most important data needed as input for the site-scale hydrological model of the unsaturated zone. The difficult and time-consuming nature of hydraulic conductivity measurements renders it infeasible to directly measure this property on large numbers of cores. Water retention and sorptivity measurements, however, can be made relatively rapidly. The sorptivity is, in principle, a unique functional of the conductivity and water retention functions. It therefore should be possible to invert sorptivity and water retention measurements in order to estimate the conductivity; the porosity is the only other parameter that is required for this inversion. In this report two methods of carrying out this inversion are presented, and are tested against a limited data set that has been collected by Flint et al. at the USGS on a set of Yucca Mountain tuffs. The absolute permeability is usually predicted by both methods to within an average error of about $0.5-1.0$ orders of magnitude. The discrepancy appears to be due to the fact that the water retention curves have only been measured during drainage, whereas the imbibition water retention curve is the one that is relevant to sorptivity measurements. Although the inversion methods also yield predictions of the relative permeability function, there are yet no unsaturated hydraulic conductivity data against which to test these predictions.

Introduction

Yucca Mountain, Nevada, is currently being studied by the U. S. Department of Energy as a potential site of an underground radioactive waste repository. The potential repository horizon is located above the water table, in a formation consisting of volcanic tuffs. As part of the site characterization process, a three-dimensional numerical hydrological model of the unsaturated zone at Yucca Mountain is being developed by scientists from Lawrence Berkeley National Laboratory, in conjunction with the U. S. Geological Survey and various other national laboratories (Wittwer et al., 1994). Among the most important data that are needed as input to this model are the hydraulic conductivity and water retention functions of the matrix rocks. Because of the spatial heterogeneity of the rocks found at Yucca Mountain, it will be necessary to measure, or otherwise determine, these hydrologic properties at many locations within the mountain. Due to the small pore sizes of most of the tuffs found at Yucca Mountain, the hydraulic conductivities are generally very low, and laboratory measurements of the hydraulic conductivity are extremely time-consuming. Hence, it would be very advantageous to be able to estimate the hydraulic conductivity from other, more readily measurable, properties. Such a method of estimating the hydraulic conductivity would also serve as a check on the measured values.

One hydraulic property that can be measured rapidly is the sorptivity, which quantifies the rate of imbibition during a one-dimensional imbibition experiment into a core that is initially only partly saturated. The sorptivity is jointly controlled and determined by the hydraulic conductivity and water retention functions. In principle, knowledge of any two of these three functions would enable the third to be determined. In this report we present two methods for estimating the hydraulic conductivity function from sorptivity and water retention measurements, and test these methods against data on seven Yucca Mountain tuff cores that have been collected by Flint et al. (1995). We note, however, that this particular data set is neither

sufficiently extensive nor accurate enough to provide a definitive test of the inversion procedures proposed in this report.

Richards Equation for One-Dimensional Imbibition

The governing equation for one-dimensional isothermal flow of liquid water in a partially saturated (also called ''unsaturated'') porous medium, in the absence of trapped gas, is the Richards equation (Hillel, 1980):

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

In the Richards equation, k, with dimensions of $[L^2]$, is the absolute (or saturated) permeability; this is the permeability of the medium to water under conditions of full liquid saturation. The permeability is essentially equivalent to the hydraulic conductivity $K = \rho g k/\mu$, because the liquid density ρ, the gravitational acceleration g, and the liquid viscosity μ are essentially constant. $k_r(S)$ is the dimensionless relative permeability function, which quantifies the extent to which partial saturation with air lowers the permeability of the rock to the liquid phase. μ, with dimensions of $[ML^{-1}T^{-1}]$, is the viscosity of the water. ψ, with dimensions of $[ML^{-1}T^{-2}]$, is the capillary (or ''matric'') potential of the water in the porous medium. S is the dimensionless liquid saturation, which is defined as the volumetric water content, θ, divided by the porosity, ϕ. The two functions $\psi(S)$ and $k_r(S)$ are often referred to as the characteristic functions of the porous medium. Note that when modeling core-scale imbibition experiments on low permeability tuffs, it is appropriate to ignore the gravitational term that is present in the more general form of the Richards equation (see Zimmerman et al., 1990,1995).

When mathematically analyzing eq. (1), it is convenient to rewrite it in a form that explicitly shows that it is a diffusion-type equation. Use of the chain rule of differentiation yields (Brutsaert, 1976)

$$\frac{\partial}{\partial x}\left[\frac{kk_r(S)}{\mu}\frac{d\psi}{dx}\right]=\frac{\partial}{\partial x}\left[\frac{kk_r(S)}{\mu}\frac{d\psi}{dS}\frac{\partial S}{\partial x}\right]=\phi\frac{\partial S}{\partial t}\ ,$$

$$\text{or}\quad \frac{\partial}{\partial x}\left[D(S)\frac{\partial S}{\partial x}\right]=\frac{\partial S}{\partial t}\ , \tag{1b}$$

where the hydraulic diffusivity for unsaturated flow is given by

$$D(S)=\frac{kk_r(S)}{\mu\phi}\frac{d\psi}{dS}\ . \tag{2}$$

The mathematical problem of one-dimensional absorption is fully-specified by augmenting eq. (1) with the following boundary/initial conditions:

$$\psi(x,t=0)=\psi_i\ , \tag{3a}$$

$$\psi(x=0,t>0)=\psi_s\ . \tag{3b}$$

Eq. (3a) states that the potential is initially equal to some value ψ_i. Aside from the small gravitational gradient, which we ignore, this represents a core that is initially at equilibrium. The potential ψ_s is the potential applied at the wetted boundary of the core. The two potentials ψ_i and ψ_s are related to the saturation S_i and S_s through the

main branch of the water retention relation $\psi(S)$. The boundary condition used in the sorptivity experiments of Flint et al. (1995) is $\psi_s = 0$, which usually corresponds to $S_s = 1.0$, which is to say full liquid saturation.

Eq. (1) governing the capillary-driven absorption of water into a porous medium is in general highly nonlinear. The nonlinearity enters the equation through the two characteristic functions, $k_r(S)$ and $\psi(S)$. For those sets of characteristic functions that have been shown to accurately model the behavior of soils or rocks, eq. (1) is not solvable in closed-form. If it were possible to develop closed-form solutions that had explicit dependences on the parameters that appear in the characteristic functions, we could then invert the experimental data to determine these parameters. Inversion of the experimental data could also be accomplished by fitting the data to numerical solutions of the governing equation. This approach has occasionally been pursued (Zachmann et al., 1981; Kool et al., 1985; Finsterle and Pruess, 1995), but involves extensive computations. Furthermore, as the sorptivity can be measured without having to determine the details of the saturation or pressure profile, it would seem that inversion methods could be devised that do not require repeated numerical solutions of the full governing differential equation.

We have taken two approaches to this inversion problem. The first is to assume that the characteristic functions are of the van Genuchten - Mualem (Mualem, 1976; van Genuchten, 1980) form, and then develop an approximate expression for the sorptivity as a function of parameters that appear in the characteristic functions. These parameters can then be found by fitting the approximate expressions to the sorptivity data. The other approach is based on the assumption that the sorptivity is a linear function of the initial saturation, which implies that the diffusivity is constant. In this case the hydraulic conductivity can be inferred directly from the measured water retention function, using eq. (2). In this report, both of these methods are applied to data that has been collected by Flint et al. (1995) on Yucca Mountain tuffs.

Sorptivity-Saturation Relationship

As the Richards equation (1) is a one-dimensional diffusion equation, its solution for the boundary/initial conditions given by eqs. (2,3) can be expressed in terms of the Boltzmann similarity variable, $\eta = x/\sqrt{t}$ (see Hillel, 1980, p. 208; Hill, 1992). One consequence of this similarity behavior is that the cumulative volumetric influx into the medium, $I(t)$, which has dimensions of [L^3], will be proportional to $t^{1/2}$, regardless of the specific form of the characteristic functions (Gardner and Mayhugh, 1958; Zimmerman et al., 1995). The constant of proportionality was called the ''sorptivity'' by Philip (1955), and denoted by **S**, so that

$$I(t) = A\mathbf{S}t^{1/2} , \tag{4}$$

where A is the surface area of the wetted boundary. This $\sqrt{t}$ dependence holds only prior to the time at which the wetting front begins to interact with the far boundary of the core, at $x = L$, after which the cumulative flux asymptotically levels off to the value $I_\infty = AL\phi(S_s - S_i)$.

The sorptivity will depend on the hydraulic properties of the porous medium, as well as on its initial saturation. The sorptivity can be found (mathematically) by solving the Richards equation by analytical or numerical means. Analytical solutions are not feasible for commonly-used characteristic functions such as those of Mualem (1976) and van Genuchten (1980), and numerical solutions do not display the manner in which the sorptivity depends on the parameters that appear in the characteristic functions. One approach that can be used to develop closed-form, albeit approximate, solutions is the integral method (Goodman, 1964). Another approach is to appeal to one of the numerous sorptivity approximations that have been proposed, which express the sorptivity as an integral functional of the diffusivity. One of the simplest of these is the approximation proposed by Philip (1955):

$$\mathbf{S}^2(S_i) = \frac{8\phi^2}{\pi} \int_{S_i}^{S_s} (S - S_i) D(S) dS \ . \tag{5}$$

According to eq. (5), the sorptivity of the soil at an initial saturation S_i depends on the hydraulic diffusivity of that soil over the range of saturations from S_i to S_s. This is to be expected, as the saturation profile will vary from S_s at the wetted boundary to S_i slightly ahead of the wetting front. In an extensive numerical study of the applicability of various sorptivity approximations to soils having diffusivities of the form $D(S) = D_o \exp(\beta S)$, Kutílek and Valentová (1986) found that eq. (5) is reasonably accurate.

Van Genuchten - Mualem Characteristic Functions

The characteristic functions that have been most widely used within the Yucca Mountain Project are those proposed by Mualem (1976) and van Genuchten (1980), which have the form

$$\psi(S) = \frac{1}{\alpha}(\hat{S}^{-1/m} - 1)^{1/n} \ , \tag{6}$$

$$k_r(S) = \hat{S}^{1/2}[1 - (1 - \hat{S}^{1/m})^m]^2 , \tag{7}$$

where $\hat{S} = (S - S_r)/(S_s - S_r)$, α is a parameter that has dimensions of inverse pressure, i.e., $[M^{-1}L^1T^2]$, and m and n are dimensionless parameters that are related by $m = 1 - 1/n$. The parameter α is, in some rough sense, proportional to the mean pore size of the rock. The parameter n is inversely related to the broadness of the pore-size distribution, in the sense that smaller values of n are associated with broader distributions, and vice versa. S_r is the ''residual'' saturation at which the liquid phase

becomes practically immobile. If eq. (6) is used to fit drainage data, the parameter S_s, which is the saturation at which the matric potential goes to zero, is usually very close to 1.0.

Zimmerman and Bodvarsson (1989) used the integral method (see Goodman, 1964) to find the following approximate expression for the sorptivity of a van Genuchten medium:

$$\mathbf{S}(S_i) = \left[\frac{2nk\phi(S_s - S_r)}{\alpha(n+1)\mu m^{1/n}} \left[\frac{S_s - S_i}{S_s - S_r} \right]^{1+1/n} \right]^{1/2} . \tag{8}$$

Eq. (8) becomes increasingly accurate for larger values of n, and for high initial saturations (see Zimmerman and Bodvarsson, 1995), but it is not uniformly accurate over all ranges of n and S_i. Guided by the algebraic form of eq. (8), and utilizing numerical solutions of the Richards equation, Zimmerman et al. (1995) derived the following more accurate expression for the sorptivity:

$$\mathbf{S}(S_i) = \left[\frac{2m^{4/3}k\phi(S_s - S_r)}{\alpha\mu} \right]^{1/2} \left[\frac{S_s - S_i}{S_s - S_r} \right]^{0.62 - 0.12m} . \tag{9}$$

As m can vary (at most) from 0 to 1, the exponent β will vary only between 0.50 and 0.62. In other words, the exponent is not very sensitive to m. As we are interested in inverting eq. (9), it is clear that this inversion is ill-posed with respect to m. Moreover, it is much easier to estimate m by fitting the water retention data to a van Genuchten curve, as was done by Flint et al. (1995). Finally, we point out that the scatter in the sorptivity data is in most cases large enough to render meaningless any attempt to use the data to distinguish between an exponent of 0.5 and, say, 0.62. Hence, in our inversions we will replace the exponent in eq. (9) with 0.5, in all cases:

$$\mathbf{S}(S_i) = \left[\frac{2m^{4/3}k\,\phi(S_s - S_r)}{\alpha\mu}\right]^{1/2}\left[\frac{S_s - S_i}{S_s - S_r}\right]^{0.5}. \tag{10}$$

Fig. 1 shows the predictions of eq. (10), along with numerically computed values of the sorptivity, as functions of the initial saturation, for different values of n. Note that as m will be estimated from the water retention data, it is not necessary that eq. (10) be able to discern subtle differences in shape between the different curves, which depend on m. It will suffice if eq. (10) gives the correct ''magnitude'' of the sorptivity curve, which it clearly does.

Linear Sorptivity - Constant Diffusivity Approximation

Some of the sorptivity functions that have been measured by Flint and Flint (1990) on volcanic tuffs from Yucca Mountain, Nevada, have seemed to be roughly linear functions of S_i. These data can be represented by functions of the form

$$\mathbf{S}(S_i) = \mathbf{S}_{\max}\left[\frac{S_s - S_i}{S_s - S_r}\right] = \mathbf{S}_{\max}(1 - \hat{S}_i). \tag{11}$$

Sorptivities of this form cannot be accurately fit to van Genuchten-Mualem model, which leads to sorptivities that vary as $(1-S_i)^{1/2}$. A similar conclusion would hold if we attempted to use a Brooks-Corey model for the characteristic functions (see Brooks and Corey, 1966; Zimmerman and Bodvarsson, 1991). In order to fit these data, we must broaden the family of characteristic functions under consideration.

We start by examining the implications of the the result $\mathbf{S}(S_i) = \mathbf{S}_{\max}(1 - \hat{S}_i)$. We first note (Warrick and Broadbridge, 1992) that if $D(S) = D_o$, where D_o is some constant, the sorptivity will have the form $\mathbf{S} = 2\phi(S_s - S_i)\sqrt{D_o/\pi}$. Hence, a constant diffusivity is consistent with the result $\mathbf{S}(S_i) = \mathbf{S}_{\max}(1 - \hat{S}_i)$. The question next arises as

to whether or not $D(S)=D_o$ is the *only* diffusivity function that leads to a sorptivity of this form. Although we have not been able to prove that this is true, there seems to be strong evidence that it is the case. For example, if we use Philip's approximation, we can prove that a linear $\mathbf{S}(S_i)$ relationship implies that $D(S)=D_o$, as follows. If $\mathbf{S}(S_i)=\mathbf{S}_{\max}(1-\hat{S}_i)$, Philip's approximation takes the form

$$\mathbf{S}_{\max}^2\left[\frac{S_s-S_i}{S_s-S_r}\right]^2=\frac{8\phi^2}{\pi}\int_{S_i}^{S_s}(S-S_i)D(S)dS\,. \tag{12}$$

Differentiating both sides of eq. (12) with respect to S_i, and using Liebnitz' rule to account for the appearance of S_i both inside the integral and as one of the endpoints, leads to

$$-2\mathbf{S}_{\max}^2\frac{(S_s-S_i)}{(S_s-S_r)^2}=\frac{-8\phi^2}{\pi}\int_{S_i}^{S_s}D(S)dS\,, \tag{13}$$

where use has been made of the fact that the integrand goes to zero at the lower end-point, $S=S_i$. Another differentiation with respect to S_i yields

$$\frac{2\mathbf{S}_{\max}^2}{(S_s-S_r)^2}=\frac{8\phi^2}{\pi}D(S_i)\,, \tag{14}$$

which can be solved to yield

$$D(S_i)=\frac{\pi\mathbf{S}_{\max}^2}{4\phi^2(S_s-S_r)^2}\,. \tag{15}$$

Hence, according to Philip's sorptivity approximation, a diffusivity of the form $S(S_i)=\mathbf{S}_{\max}(1-\hat{S}_i)$ corresponds *uniquely* to a constant diffusivity D_o, with $\mathbf{S}_{\max}=2\phi(S_s-S_r)\sqrt{D_o/\pi}$.

Further evidence suggesting that linear sorptivities correspond only to a constant diffusivity can be found in the numerical solutions computed by Kutílek and Valentová (1986) for the family of diffusivities of the form $D(S)=D_o\exp(\beta S)$. They found that the $\mathbf{S}(S_i)$ curve is concave up for $\beta<0$, concave down for $\beta>0$, and linear only when $\beta=0$, i.e., for $D(S)=D_o$. In light of the evidence presented above, it seems reasonable to conclude that $D(S)=D_o$ is the only diffusivity function that will lead to a linear sorptivity function.

If the diffusivity is constant, eqs. (2) and (15) can be inverted to yield

$$kk_r(S) = \mu\phi D_o\left[\frac{d\psi}{dS}\right]^{-1} = \frac{\mu\pi\mathbf{S}_{\max}^2}{4\phi(S_s-S_r)^2}\left[\frac{d\psi}{dS}\right]^{-1}. \tag{16}$$

Hence, if the water retention function is known, the hydraulic conductivity function can be found from eq. (16). An advantage of this equation is that *any* water retention function that fits the data can be used; there is no restriction of the $\psi(S)$ function to any particular algebraic form. The simplest function that can be used to fit water retention data is a power-law relationship between S and ψ, as has been used by Brooks and Corey (1966) and others:

$$\psi(S) = -\psi_a\left[\frac{S-S_r}{S_s-S_r}\right]^{\gamma}, \tag{17}$$

where $-\psi_a$ is the air-entry potential; the minus sign is included so that ψ_a can be

treated as a positive number. Combining eqs. (16) and (17) leads to

$$kk_r(S) = \frac{\mu\pi \mathbf{S}_{\max}^2}{4\gamma\phi(S_s - S_r)\psi_a} S^{\gamma+1}, \tag{18}$$

from which we immediately see that that

$$k_{sat} = \frac{\mu\pi \mathbf{S}_{\max}^2}{4\gamma\phi(S_s - S_r)\psi_a}. \tag{19}$$

Inversion Procedure

The purpose of the inversion methods developed above is to enable accurate predictions of the hydraulic conductivity to be made based on sorptivity and water retention measurements. In order to test the accuracy of these methods, however, we need a data set that includes measurement of all three functions. We will analyze data from seven Yucca Mountain cores that have been collected by the USGS. Water retention measurements have been made on each of these cores (Flint et al., 1995); in most cases the data were fairly smooth, and were fit reasonably well with both van Genuchten or power-law functions. These curve fits will be used to find the pore-size parameters such as m and α. As explained in detail below, when fitting the sorptivity data we use measured values of porosity, and the inferred values of the pore-size distribution parameters, leaving only one parameter, such as $\mathbf{S}_{\max}$, as a fitting parameter. Although there is typically much scatter in the sorptivity-saturation data, if we assume that the scatter is due to random experimental errors, rather than some systematic bias, it seems $\mathbf{S}_{\max}$ is probably accurate to within $\pm 50\%$ (see Figs. 2-8). As the conductivity predictions depend on $\mathbf{S}_{\max}^2$, the uncertainty in $\mathbf{S}_{\max}$ will lead to an uncertainty of

a factor of two in our conductivity predictions; this is in addition to any uncertainty stemming from the the water retention data. Zimmerman et al. (1993) tested the inversion method that was based on the linear-sorptivity model on one vitrified tuff from the Calico Hills unit, and found reasonable agreement with measured conductivities over a range of saturations from $0.4-1.0$. The seven cores discussed below have only had their conductivities measured at $S=1.0$, i.e., $k \equiv k_{sat}$. Our inversion methods will therefore only be tested as to their predictions of the saturated conductivity. To simplify the inversion procedures, we will take $S_s=1.0$ and $S_r=0$ for each specimen, although finite values of S_r have been measured by Flint et al. (1995). In all cases, S_r was less than 0.10. As the predicted values of k will depend on $(S_s-S_r)^2$, the effect of neglecting the finite value of S_r will be negligible compared to other sources of uncertainty.

One factor that must be accounted for when performing the inversions is that, in some cores, the saturation behind the wetting front (i.e., at $x=0$) did not reach 100%. This saturation, S_{bwf}, can be estimated by performing a mass balance on the raw imbibition data, as described below. The permeability k that appears in the sorptivity equation (11) is intended to represent the conductivity behind the wetting front. Hence, we can account for the fact that $S_{bwf}<1$ by replacing k with $k_{sat}k_r(S=S_{bwf})$. This procedure is not exact, for the following reason. The potential behind the wetting front is $\psi_{bwf}=0$, so we see that S_{bwf} and ψ_{bwf} are *not* related to each other through the van Genuchten water retention function (6). This is because eq. (6) is the *drainage* branch of the water retention relation, whereas the relevant portion of the water retention relation during a sorptivity measurement is the *imbibition* curve. Porous rocks such as tuffs often exhibit hysteresis in their water retention relations, in the sense that drainage and imbibition do not follow the same curves (see Niemi and Bodvarsson, 1988). A schematic of a typical hysteresis curve is shown in Fig. 9, where it is seen that, during imbibition, the saturation corresponding to zero matric potential is often

appreciably less than 1.0. As hysteresis measurements have not been made on these cores, we have little choice but to use the water retention curves that were measured during drainage to estimate parameters such as the van Genuchten α and m. However, we also assume, as is customary, that k_r is a one-to-one function of S, which is to say that there is no hysteresis in the $k_r(S)$ curve.

Van Genuchten Model

Our van Genuchten inversions are based on the following version of eq. (11), with $S_s = 1.0$ and $S_r = 0$, but with k replaced by $k_{sat} k_r(S_{bwf})$, as explained above:

$$\mathbf{S}(S_i) = \left[\frac{2m^{4/3} k_{sat} k_r(S_{bwf}) \phi}{\alpha \mu} \right]^{1/2} (1 - S_i)^{0.5} = \mathbf{S}_{\max}(1 - S_i)^{0.5}. \tag{20}$$

We fit the measured sorptivities to the function $\mathbf{S} = \mathbf{S}_{\max}(1 - S_i)^{0.5}$, with $\mathbf{S}_{\max}$ as the fitting parameter. With m and α taken from the curve fit to the water retention data performed by Flint et al. (1995), and using the measured porosity and a room-temperature water viscosity of 1.0×10^{-3} Pa s, we find a predicted permeability behind the wetting front of

$$k_{sat} k_r(S_{bwf}) = \frac{\alpha \mu \mathbf{S}_{\max}^2}{2m^{4/3} \phi}. \tag{21}$$

The predicted saturated permeability is then found by dividing by $k_r(S_{bwf})$, where the relative permeability function $k_r(S)$ is taken from eq. (7):

$$k_{sat} = \frac{\alpha \mu \mathbf{S}_{\max}^2}{2m^{4/3} \phi k_r(S_{bwf})}. \tag{22}$$

Linear Sorptivity Model

To carry out the inversions based on the linear sorptivity model, we need a functional form for the water retention curve. We will use the Brooks-Corey water retention curve-fits that were calculated by Flint et al. (1995), because they are essentially power-law functions, and have a simpler form than the van Genuchten equation. If we again set $S_s = 1.0$ and $S_r = 0$, and identify k with $k_{sat} k_r(S_{bwf})$, eq. (19) takes the form

$$k_{sat} k_r(S_{bwf}) = \frac{\mu \pi \mathbf{S}_{\max}^2}{4\gamma\phi\psi_a}. \tag{23}$$

which can be solved for

$$k_{sat} = \frac{\mu \pi \mathbf{S}_{\max}^2}{4\gamma\phi\psi_a k_r(S_{bwf})} = \frac{\mu \pi \mathbf{S}_{\max}^2}{4\gamma\phi\psi_a} S_{bwf}^{-(1+\gamma)}. \tag{24}$$

Note that ψ_a plays a role as a characteristic potential that is somewhat analogous to $1/\alpha$ in the van Genuchten model. The van Genuchten parameter $n = 1/(1-m)$ can be related to γ by noting that, at low saturations, eq. (6) takes the form $\psi = (1/\alpha)\hat{S}^{-(n-1)}$, which shows that γ is analogous to $n-1$. Hence, we see that the predictions of the two models, given by eqs. (19) and (24), are actually quite similar.

Permeability Predictions and Comparison with Measured Data

The measured sorptivities of the seven samples are shown in Figs. 2-8. The sorptivity was usually measured at six different initial saturations. However, at high values of S_i it was often not possible to determine the sorptivity from the imbibition data, as the I *vs.* $\sqrt{t}$ curves did not exhibit a clear straight-line region at small times. This is because the wetting front becomes very diffuse when S_i is close to 1.0 (see

Zimmerman and Bodvarsson, 1989), and so the effect of the far boundary at $x = L$ begins to influence the imbibition rate at relatively early times. For the purposes of the curve fits, we added in an additional point $\{\mathbf{S} = 0, S_i = 1.0\}$, as the sorptivity must be zero when the rock is initially at full saturation. The sorptivities of four of the seven samples were fit more closely with a linear sorptivity-saturation function, eq. (12), whereas the other three were fitted more accurately with the van Genuchten model, eq. (17). The samples that exhibited nearly linear relationships between sorptivity and initial saturation tended to be those with lower porosities. For each sample, the maximum sorptivities $\mathbf{S}_{\max}$ corresponding to the two types of curve fits differed by about $15-25\%$.

The saturation behind the wetting front was calculated by assuming that the saturation in the core asymptotically reaches a uniform level, S_{bwf}, as $t \to \infty$. If the asymptotic cumulative volumetric imbibition is denoted by I_∞, then S_{bwf} is found from

$$S_{bwf} = S_i + \frac{I_\infty}{AL\phi}, \tag{25}$$

where A is the cross-sectional area of the core, L is the length of the core, ϕ is the porosity, and S_i is the initial saturation. In general, S_{bwf} will depend on the initial saturation; for example, as $S_i \to 1.0$, S_{bwf} must also approach 1.0. For each core we calculate a single value of S_{bwf}, using the data from the imbibition tests that were conducted on cores that were initially totally dry, i.e., $S_i = 0$, This initial saturation was used for two reasons, one being that I_∞ will be a maximum for $S_i = 0$, so small absolute errors in estimating I_∞ will lead to smaller relative errors in the estimate of S_{bwf}. Another reason is that, in many cases, the curve fits were somewhat more accurate at $S_i = 0$ than at intermediate values of S_i.

For samples BB13A, BB68, and CH47, the value of S_{bwf} calculated from eq. (25) was somewhat greater than 1.0; we attribute this to experimental error, and set $S_{bwf} = 1.0$. In these cases, the term $k_r(S_{bwf})$ in the denominator of eq. (22) was set equal to 1.0 when calculating k_{sat}. The values of S_{bwf} estimated for the other four cores were each in the range of $0.5-0.6$ (see Table 1). The predicted values of k_{sat} are shown in Table 1. Measured values of k_{sat} are given by Flint et al. (1995) for five of the samples. For the other two, BB13A and BB68, we estimated k_{sat} using the regression equations for k_{sat} as a function of porosity that were developed by Flint et al. (1995) based on a large number (a few dozen) measurements on cores taken from rock outcrops at Yucca Mountain. These regressions were accurate (on average) to within about one order of magnitude, although in some cases the errors were as large as $2-3$ orders of magnitude. The mean of the absolute value of the error in log k_{sat} was 0.7 for the van Genuchten inversions, and 1.1 for the inversion based on the linear sorptivity model. The van Genuchten inversion tended to be more accurate for those cores whose sorptivities were fit more closely by the van Genuchten model (BT17, BT3V, and BT11) than by the linear sorptivity model, and *vice versa*. If in each case we use the prediction based on the model that provided the best fit to the sorptivity, the mean error in log k_{sat} is about 0.6, which corresponds to a factor of four in k_{sat} itself. This may well be within the error bars of the conductivity measurements performed by Flint et al. (1995).

Discussion and Conclusions

As part of the process of characterizing the suitability of Yucca Mountain as a potential location of an underground radioactive waste repository, a detailed three-dimensional numerical model is being constructed to study the hydrological behavior of the unsaturated zone (Wittwer et al., 1994). In order for the model to be as realistic as possible, accurate hydrological data are needed for the various geological strata.

The numerical model requires water retention and hydraulic conductivity 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. As mentioned above, it is very difficult and time-consuming to make accurate measurements of hydraulic conductivity curves on the relatively impermeable volcanic tuffs that are found at Yucca Mountain. Sorptivity measurements, on the other hand, can be made relatively quickly and accurately.

We have presented two methods of estimating the hydraulic conductivity function from sorptivity and water retention data. Both methods have been seen to yield reasonable, although not extremely accurate, predictions of the saturated permeability. The main source of error in the predictions is probably the fact that the water retention curves were measured during drainage, whereas the imbibition water retention curve is actually the relevant curve for modeling sorptivity experiments. Measurements of the imbibition water retention curves would therefore seem to be needed for more accurate predictions. Moreover, the imbibition (rather than drainage) curves are the ones that are relevant to fracture/matrix flow that will occur during transient infiltration processes at Yucca Mountain, and which will control the time required for water to reach the water table. We note also that unsaturated hydraulic conductivity measurements have been made on very few cores from Yucca Mountain. Such data are needed to test our predictions of the relative permeability function. However, we point out that the relative permeability function $k_r(S)$ is in fact used in our inversion procedure to find k_{sat}, as eq. (22) shows. In the absence of saturated hydraulic conductivity measurements, our proposed inversion procedure can be used to give estimates of the matrix properties that are needed as input to the site-scale hydrologic model.

Acknowledgements

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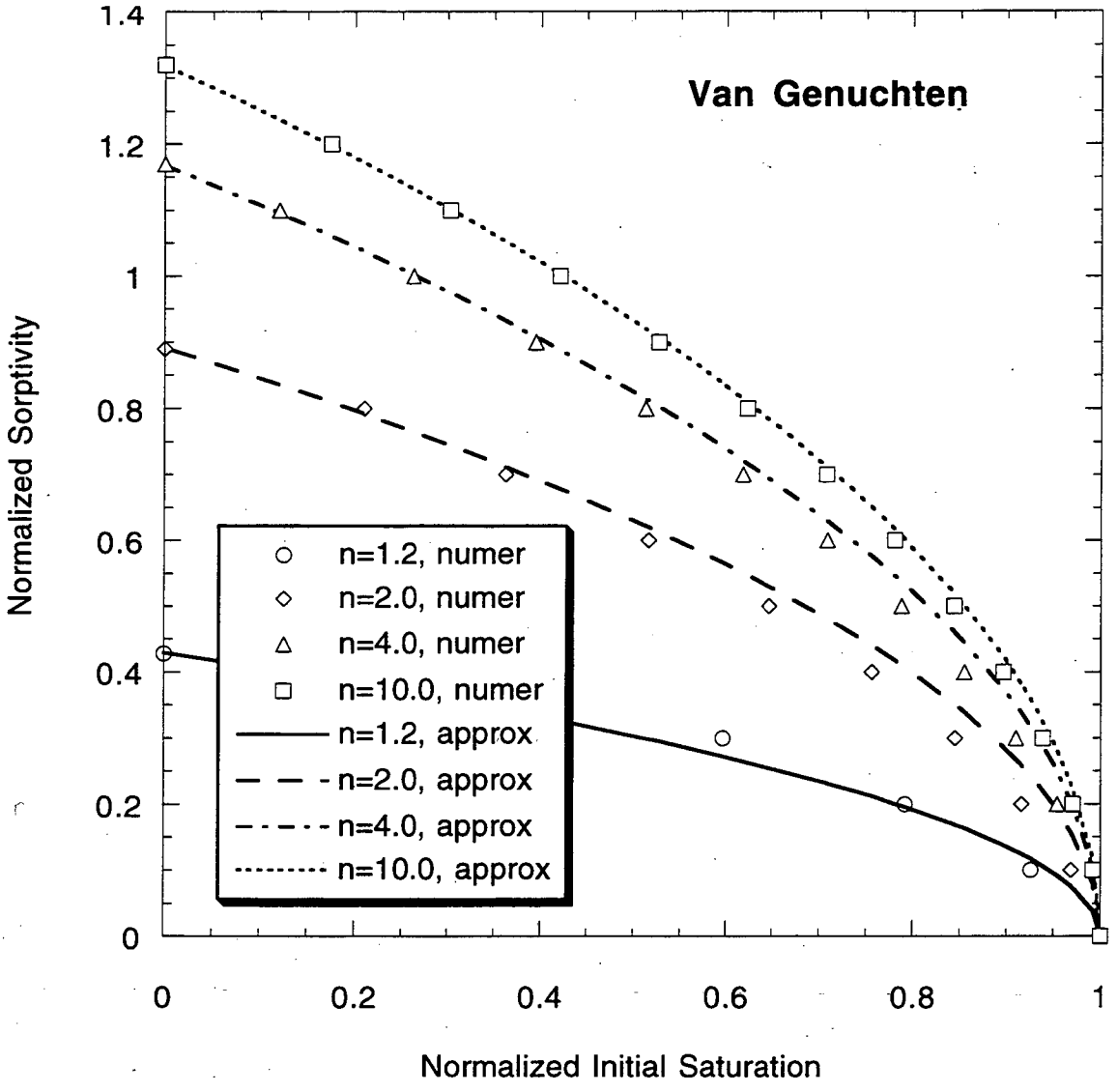
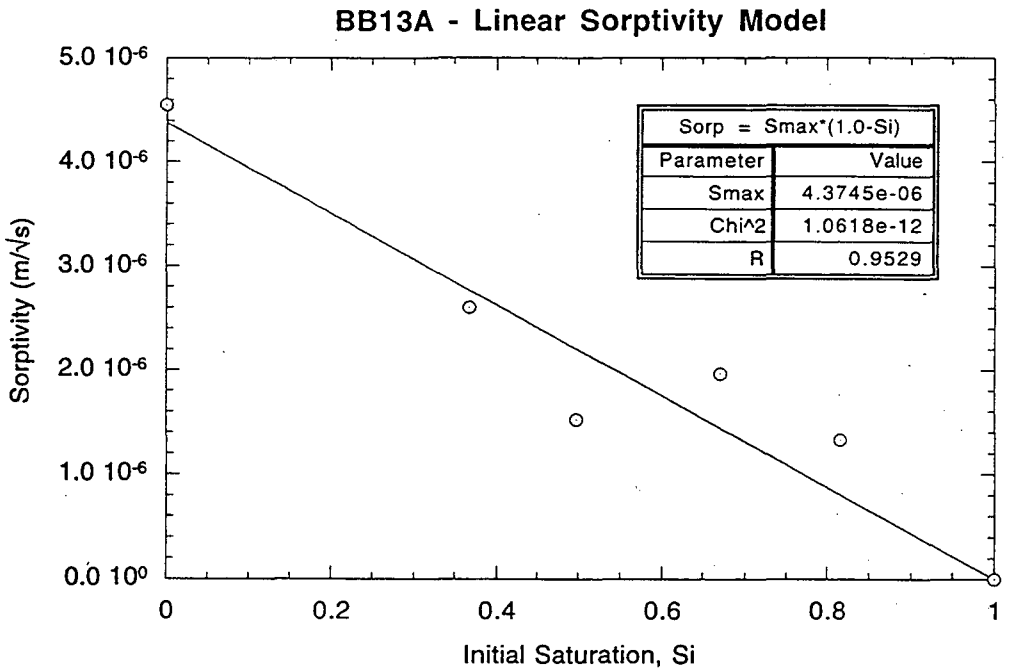


Fig. 1. Sorptivity of a van Genuchten medium, as a function of initial saturation, for various values of the parameter n. The normalized sorptivity is defined by $[\alpha\mu/k\,\phi(S_s-S_r)]^{1/2}\mathbf{S}$; the normalized initial saturation is defined by $\hat{S}_i=(S_i-S_r)/(S_s-S_r)$. The curves are generated from eq. (11); the symbols are values computed by numerically solving eqs. (1-3).



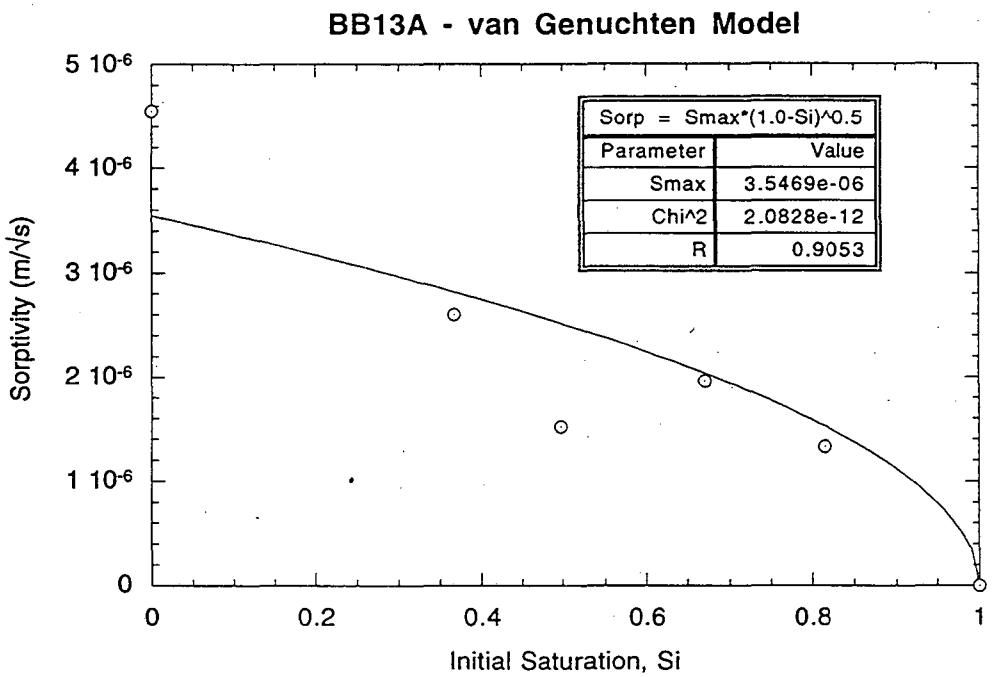
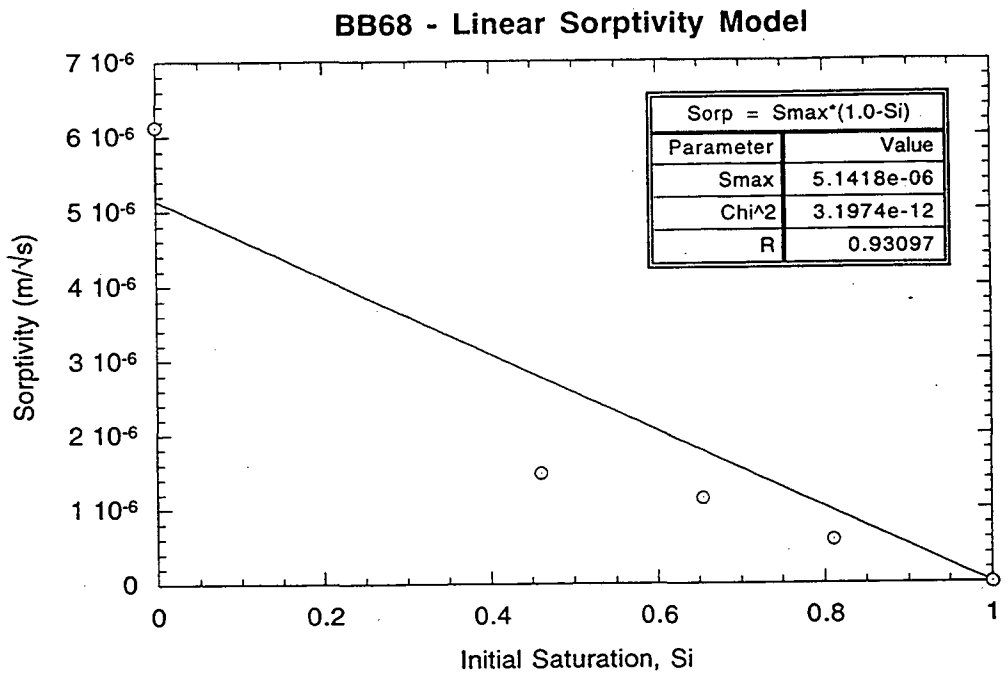


Fig. 2. Sorptivities of sample BB13A, a mottled tuff from the Topopah Spring member. The top graph shows the results of a fit to the linear sorptivity model, the bottom graph shows the results of a fit to the van Genuchten model, eq. (20).



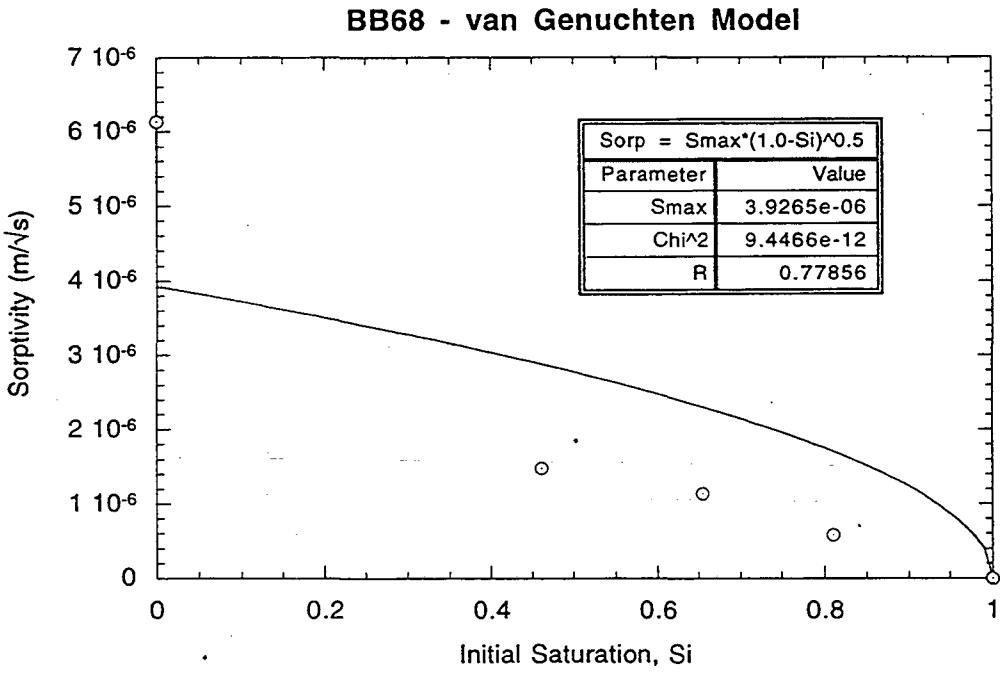
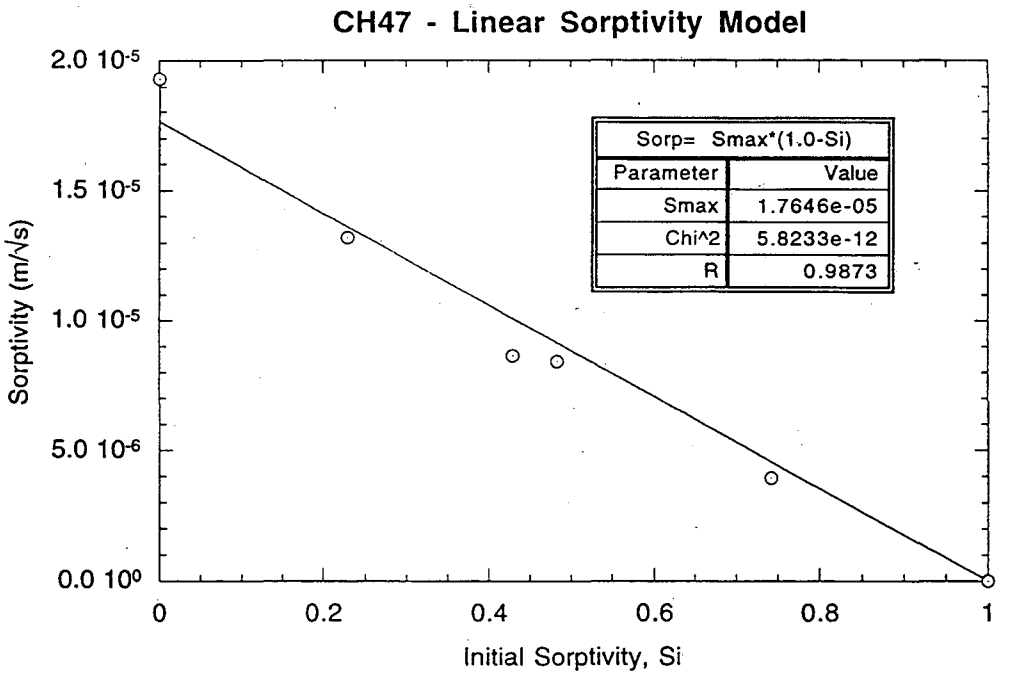


Fig. 3. Sorptivities of sample BB68, a tuff from the upper lithophysal zone of the Topopah Spring member. The top graph shows the results of a fit to the linear sorptivity model, the bottom graph shows the results of a fit to the van Genuchten model, eq. (20).



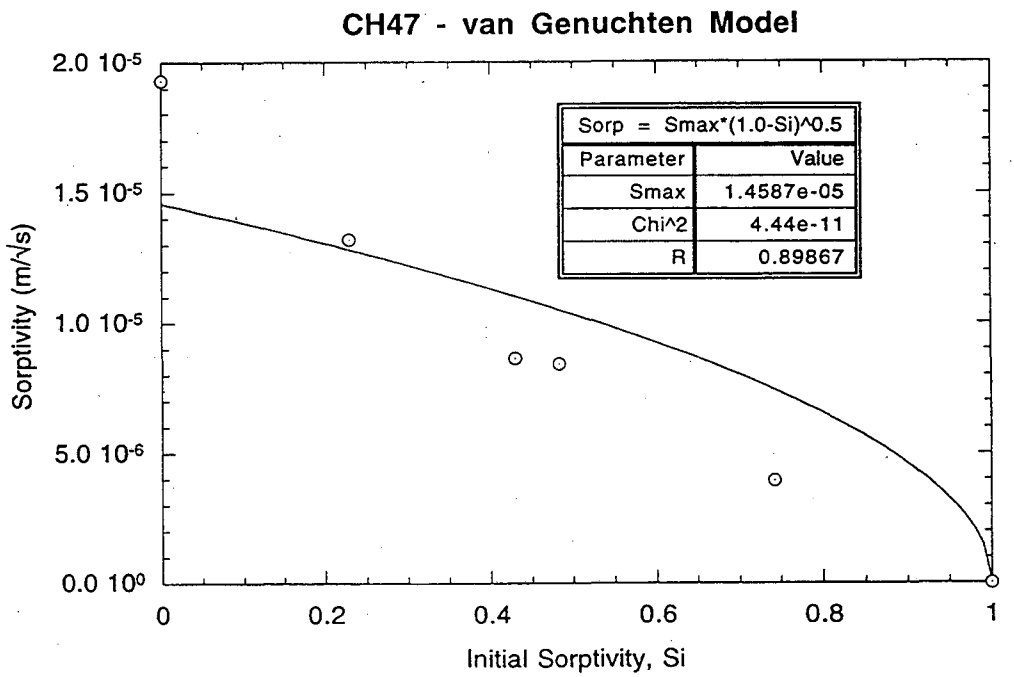
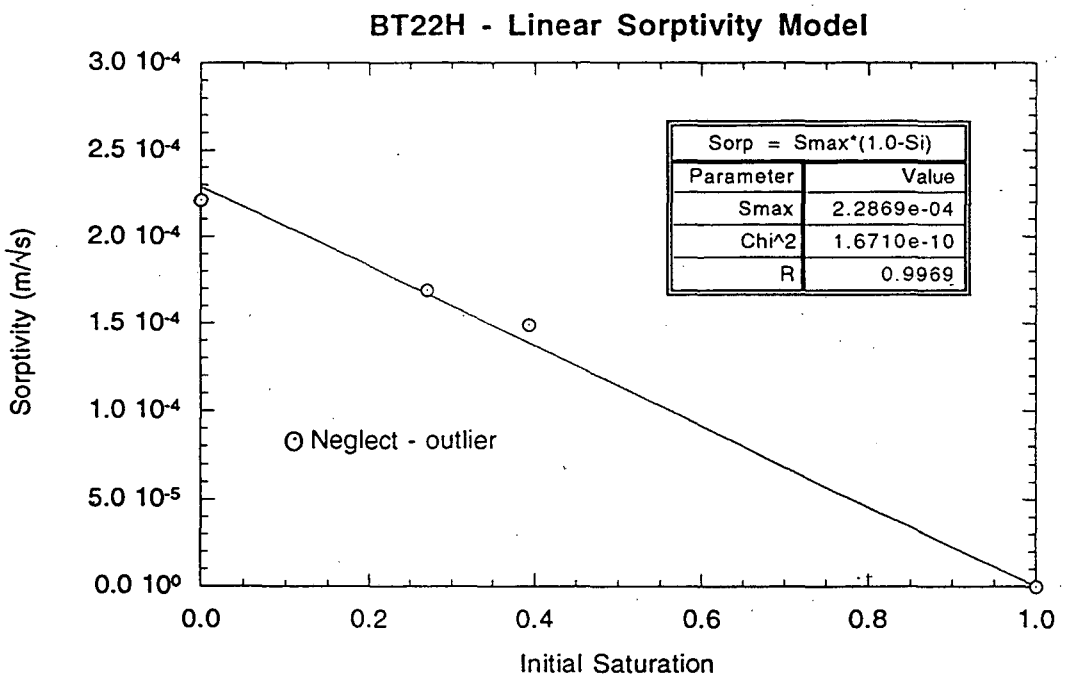


Fig. 4. Sorptivities of sample CH47, a zeolitized tuff from the Calico Hills member. The top graph shows the results of a fit to the linear sorptivity model, the bottom graph shows the results of a fit to the van Genuchten model, eq. (20).



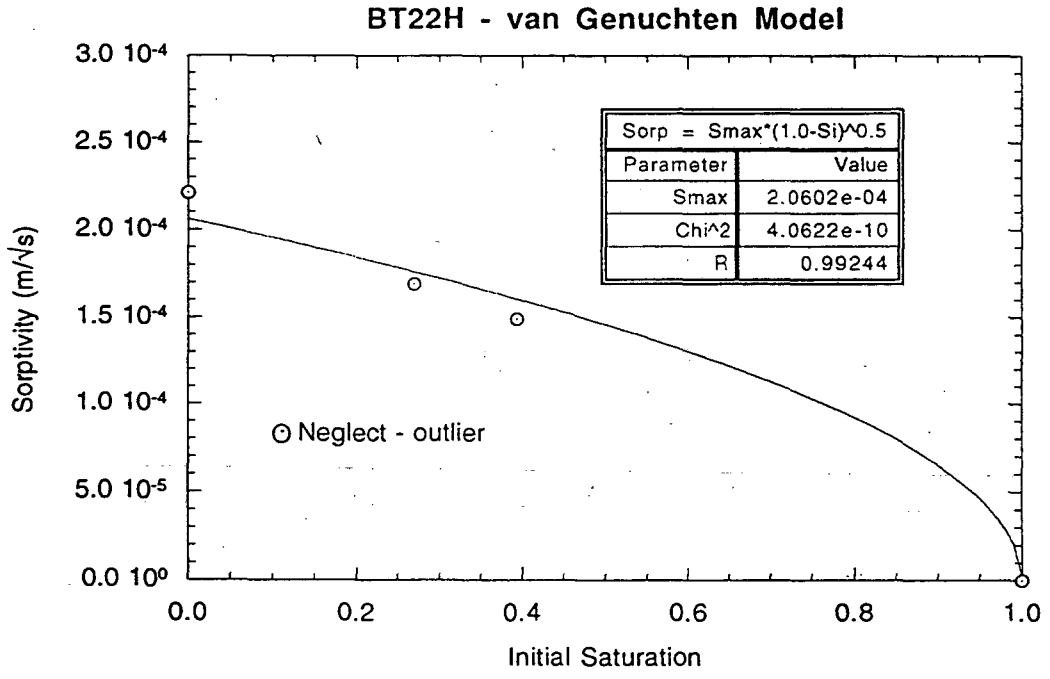
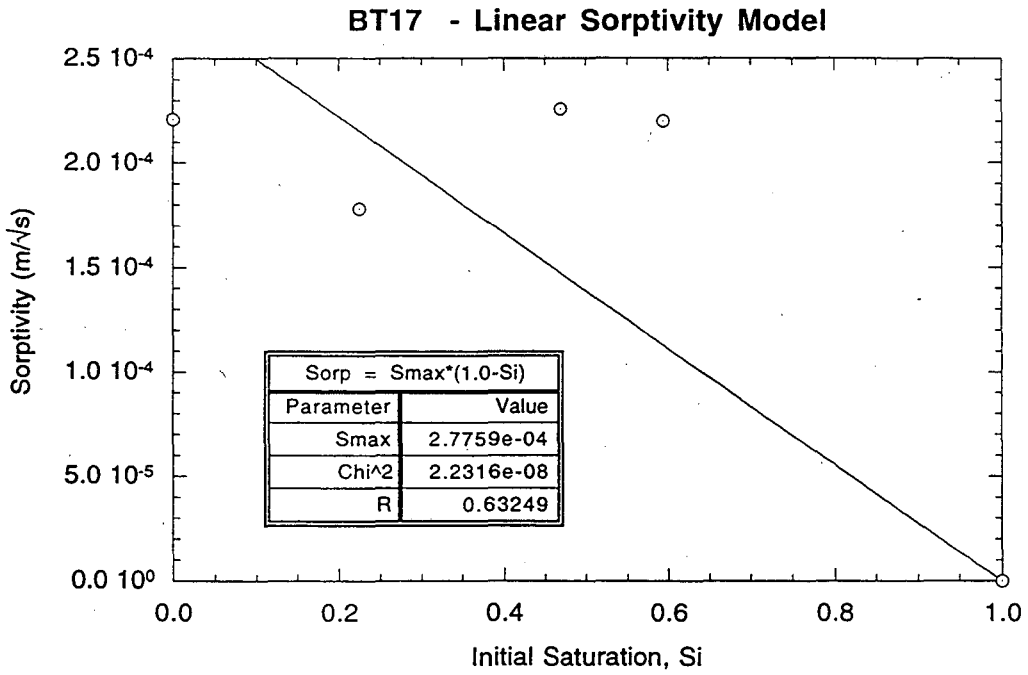


Fig. 5. Sorptivities of sample BT22H, a tuff from the shardy base of the Tiva Canyon member. The top graph shows the results of a fit to the linear sorptivity model, the bottom graph shows the results of a fit to the van Genuchten model, eq. (20).



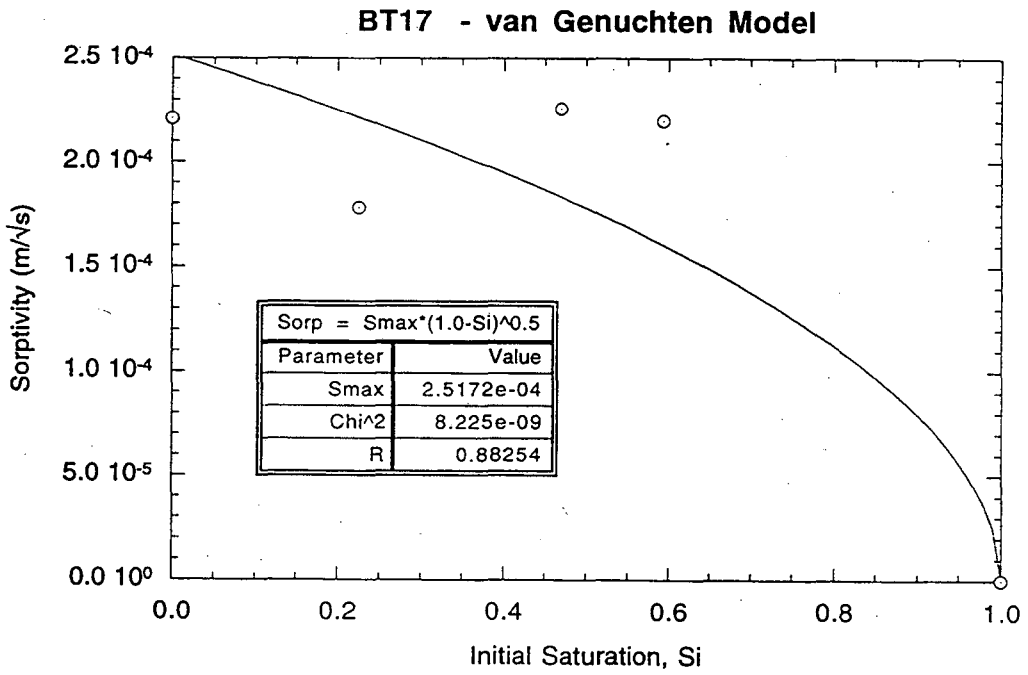
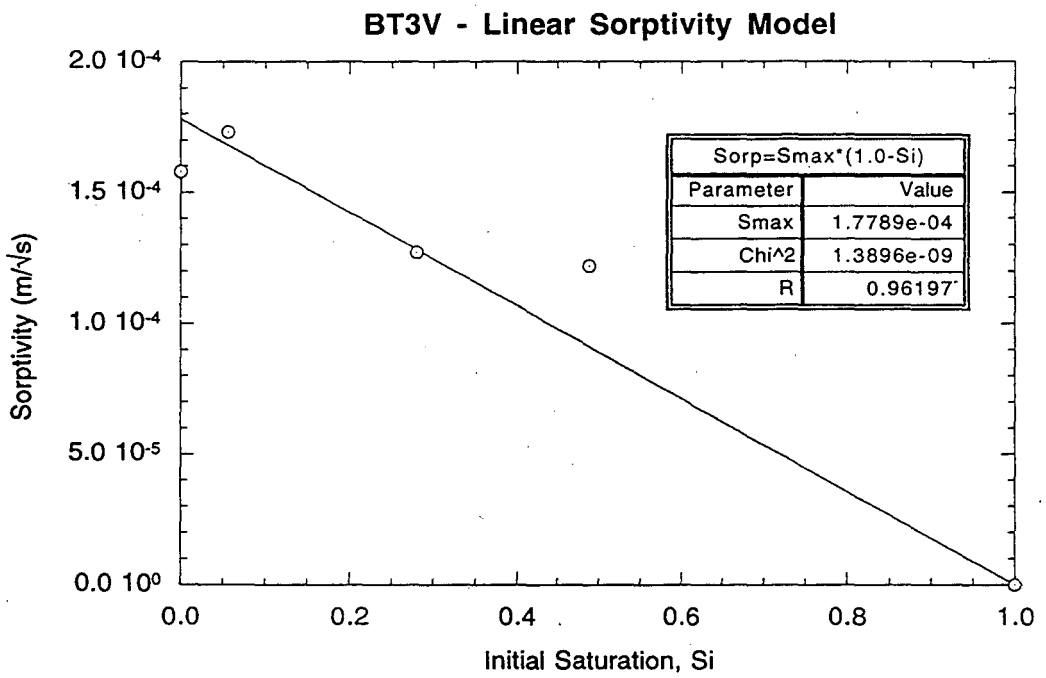


Fig. 6. Sorptivities of sample BT17, a tuff from the Yucca Mountain member. The top graph shows the results of a fit to the linear sorptivity model, the bottom graph shows the results of a fit to the van Genuchten model, eq. (20).



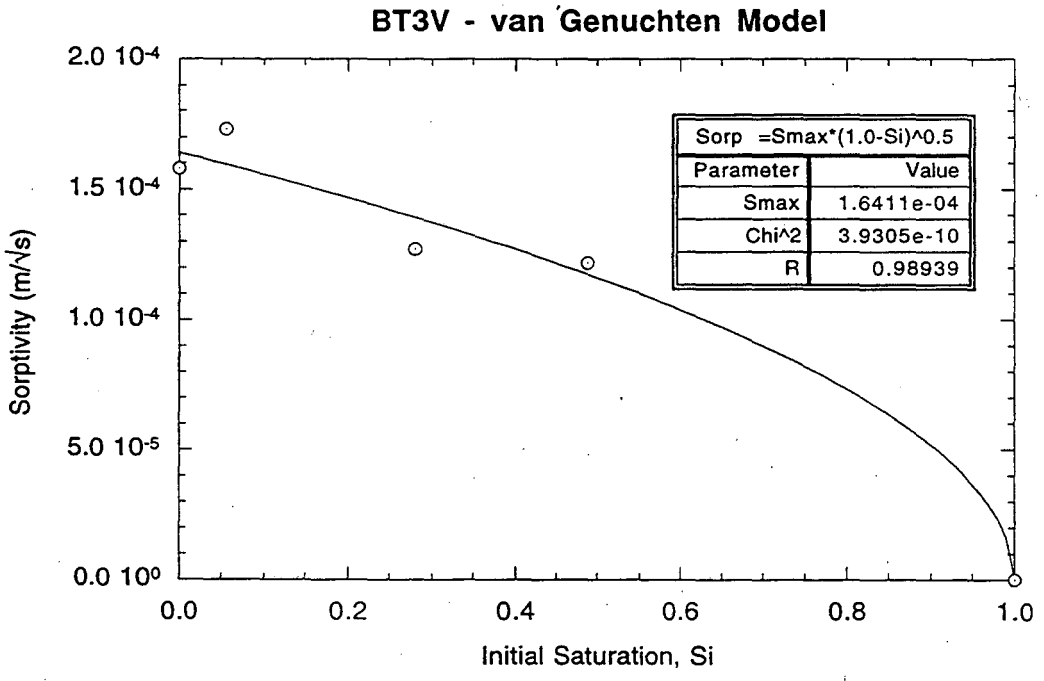
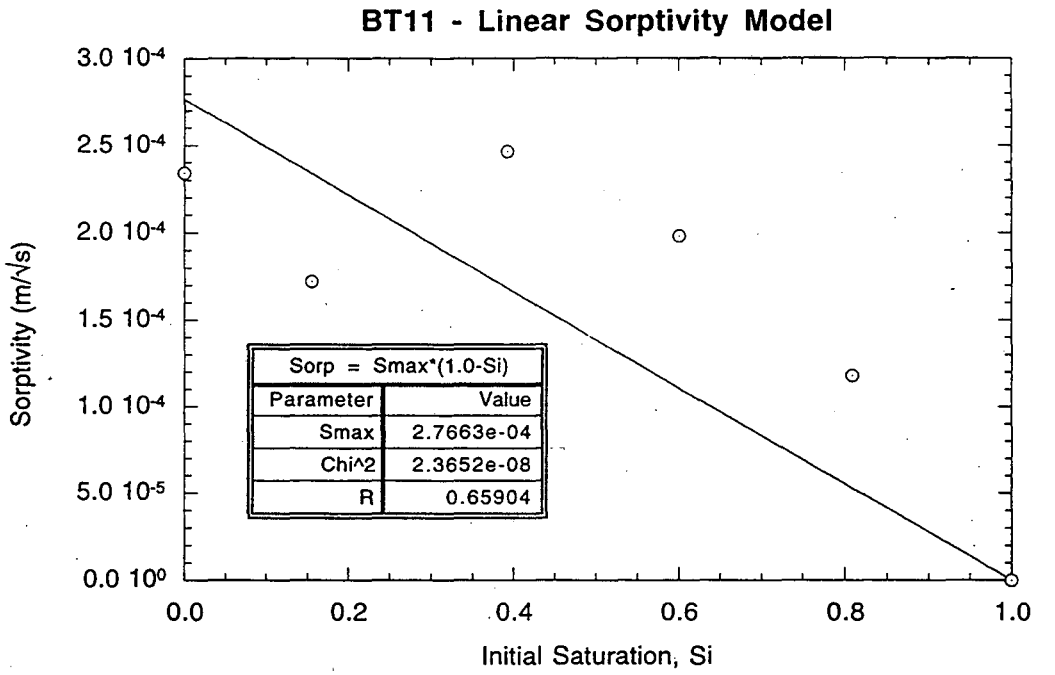


Fig. 7. Sorptivities of sample BT3V, a nonwelded tuff from the Topopah Spring member. The top graph shows the results of a fit to the linear sorptivity model, the bottom graph shows the results of a fit to the van Genuchten model, eq. (20).



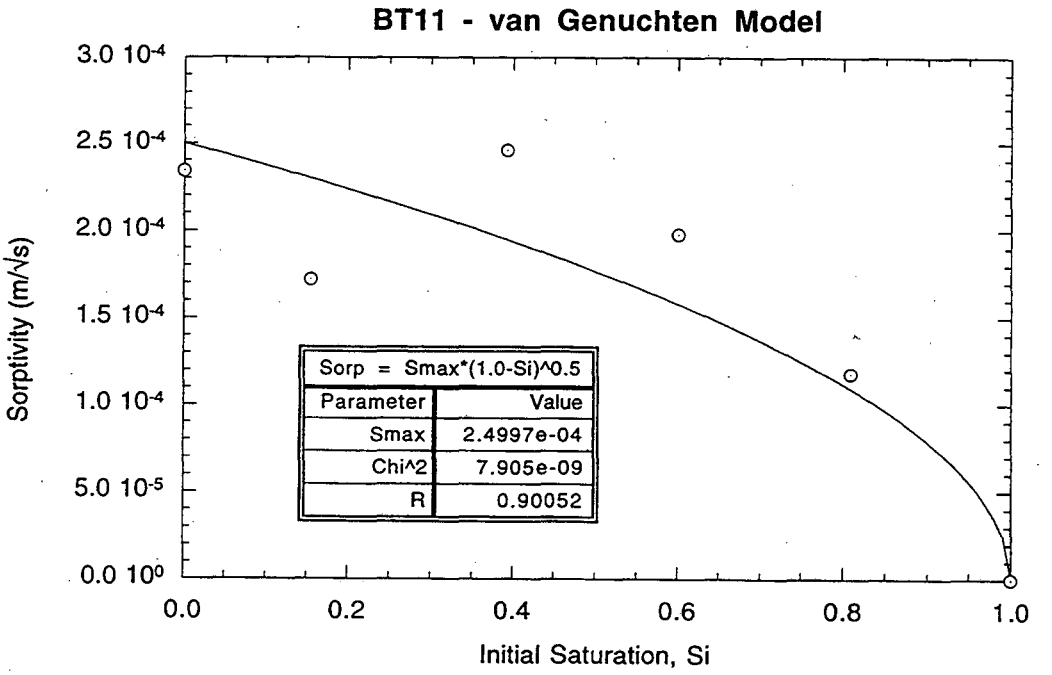


Fig. 8. Sorptivities of sample BT11, a tuff from the Pah Canyon member. The top graph shows the results of a fit to the linear sorptivity model, the bottom graph shows the results of a fit to the van Genuchten model, eq. (20).

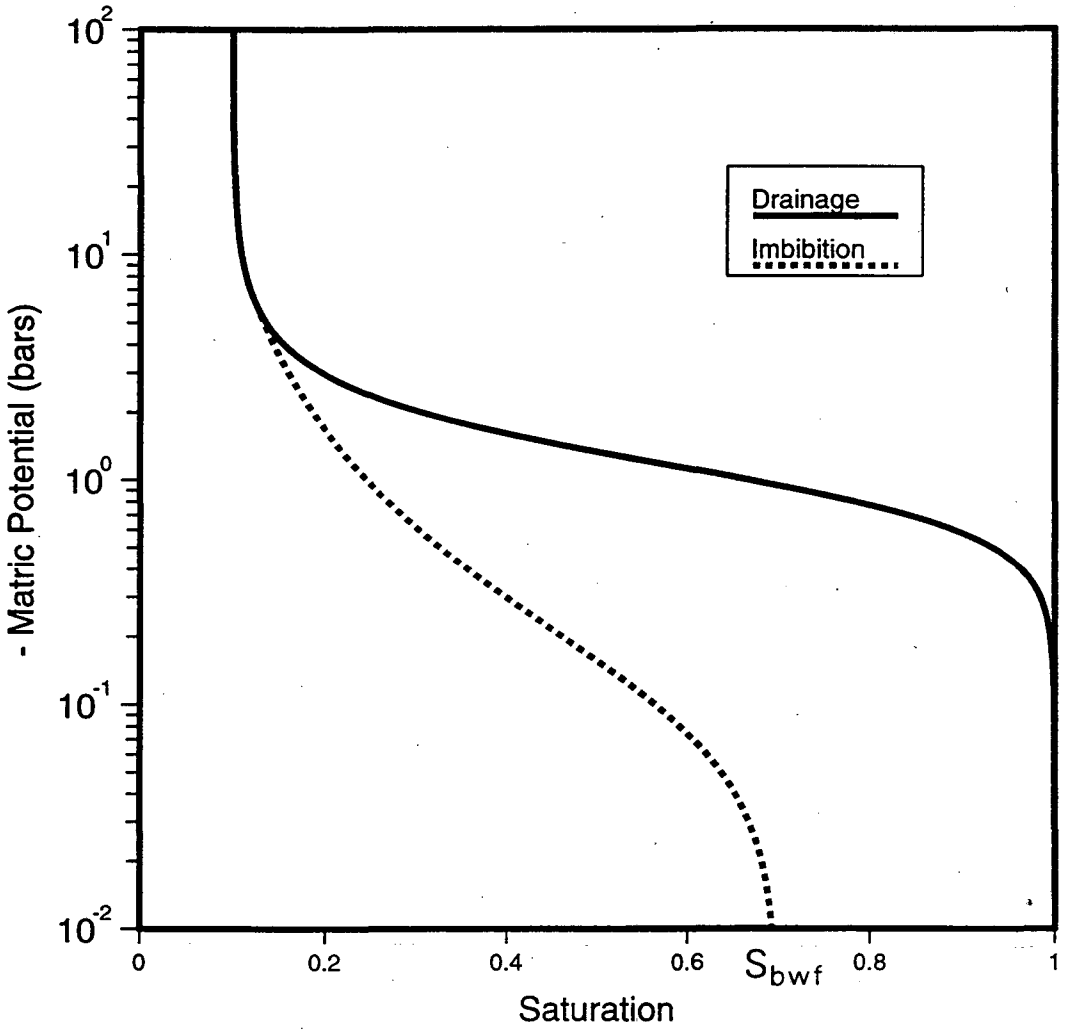


Fig. 9. Schematic drawing of typical water retention hysteresis curve (after Niemi and Bodvarsson, 1988). During drainage of water, the saturation approaches 1 as the matric potential goes to zero. During imbibition, however, the saturation will only reach S_{bwf} at zero potential, due to air being encapsulated and trapped in the core.

Table 1. Predicted values of the saturated permeabilities of seven tuffs from outcrops at Yucca Mountain. The two sets of predicted values are from the two inversion methods described in the text. The measured values are taken from Flint et al. (1995). The "measured" values for cores BB13A and BB68 are estimated from the regression curves found by Flint et al., based on a data set of a few dozen cores.

Sample	ϕ	S_{bwf}	log K_{sat} (m^2) van G model	log K_{sat} (m^2) linear model	log K_{sat} (m^2) measured
BB13A	0.06	1.00	-18.1	-18.3	-19.0
BB68	0.06	1.00	-18.5	-18.5	-19.0
CH47	0.23	1.00	-16.6	-17.9	-17.5
BT22H	0.37	0.57	-13.5	-14.0	-12.8
BT17	0.39	0.56	-13.0	-14.2	-12.5
BT3V	0.39	0.60	-13.7	-14.3	-13.3
BT11	0.57	0.58	-13.6	-14.5	-12.5

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