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Introduction

Many soils contain rock fragments the sizes of which are much larger than the average pore size of the sieved soil. Due to the fact that these fragments are often fairly large in relation to the soil testing apparatus, it is common to remove them before performing hydrologic tests on the soil (Reinhart, 1961; Dunn and Mehuys, 1984). The question then arises as to whether or not there is a simple way to correct the laboratory-measured values to account for the fragments, so as to arrive at property values that can apply to the soil *in situ*. This question has arisen in the surface infiltration studies that are part of the site characterization program at Yucca Mountain, where accurate values of the hydraulic conductivities of near-surface soils are needed in order to accurately estimate infiltration rates. Although this problem has been recognized for some time, and numerous review articles have been written (Childs and Flint, 1990; Brakensiek and Rawls, 1994; Poesen and Lavee, 1994), there are as yet no proven models to account for the effect of rock fragments on hydraulic conductivity and water retention. In this report we will develop some simple physically-based models to account for the effects of rock fragments on gross hydrological properties, and apply the resulting equations to experimental data taken from the literature. These models are intended for application to data that is currently being collected by scientists from the USGS on near-surface soils from Yucca Mountain.

Overall Hydraulic Conductivity

We assume that the rock/soil mixture can be modeled as a two-component continuum (see Fig. 1). One condition that must be satisfied in order for this assumption to be justified is that the characteristic size of the rock fragments must be larger than the REV length scale of the soil (Bear, 1972). This scale, L_1, is in general assumed to be at least an order of magnitude larger than the size of the largest soil particles, which we will denote as d_p. Therefore, we will require that the characteristic size of the rock fragments, d_f, be at least an order of magnitude larger than the largest soil particles, i.e., $d_f \geq L_1 \gg d_p$. If this is the case, the soil can then be treated as a continuum on the length scale of the rock fragments. The REV scale for the soil/rock mixture is then taken to be at least an order of magnitude larger than the characteristic rock fragment size, i.e., $L_2 \gg d_f$. Another requirement for the validity of the continuum treatment of the two-component mixture is that the matric potential be nearly uniform over the length scale L_2. If the potential changes drastically over distances that are on the same order as d_f, the continuum treatment of the soil/rock mixture would not be justified. For example, during vertical infiltration it would be necessary for the wetting front to have penetrated to a depth $z \geq L_2$ in order for this approach to be valid. If all of these conditions are fulfilled, the problem is reduced to a classical effective two-component conductivity problem, in which case numerous bounds, models, etc. that were originally derived in the context of thermal or electrical conductivity are directly applicable.

We will develop a model for the effective hydraulic conductivity of a soil/rock system in the general case where both the soil and the rock have finite conductivities, although in most practical applications the conductivity of the rock fragments could be assumed to be negligible. We expect the effective hydraulic conductivity of a two-component rock/soil mixture to lie between the conductivity of the soil, K_s, and that of the rock fragments, K_r, in some proportion that depends on the relative amounts of rock and soil. This proportion is often expressed in terms of the weight (or mass) fraction of rock fragments, which is easier to measure than is the volume fraction. As particle density does not enter into the governing equations for conductivity in any way, the effective conductivity should not depend explicitly on weight fraction. However, the weight fraction may be useful in estimating the volume fraction (Flint and Childs, 1984). The rock and soil conductivities will each vary with the potential, but for the purposes of discussing effective conductivity, we must assume that ψ is essentially uniform over a certain REV. We will work in terms of the hydraulic conductivity K, which is related to the permeability k through the relation $K = \rho g k / \mu$, where ρ and μ are the density and viscosity of the pore fluid, and g is the gravitational acceleration. As these other parameters are constant at any given temperature, the equations we present for the effective conductivity apply equally well to the effective permeability.

The simplest theoretical predictions of the effective conductivity are the arithmetic and harmonic means of the two conductivities, which correspond to ''parallel'' and ''series'' models, respectively. These models yield the following effective conductivities:

$$K = cK_r + (1-c)K_s \quad \text{(arithmetic mean)}, \tag{1}$$

$$\frac{1}{K} = \frac{c}{K_r} + \frac{1-c}{K_s} \quad \text{(harmonic mean)}, \tag{2}$$

where c is the volume fraction of the rock fragments. A weighted geometric mean, $K = K_s^{1-c} K_r^c$ is sometimes used to predict the effective conductivity, although it has no particular theoretical justification, nor does it correspond to any simple geometrical model. The arithmetic and harmonic means were rigorously shown by Wiener in 1912 to be upper and lower bounds on the actual effective conductivity (see Dagan, 1989), regardless of the precise shape and distribution of the inclusions. They are not, however, the narrowest known bounds that are still independent of microstructure. The following bounds derived by Hashin and Shtrikman (1962) are always at least as restrictive as the series and parallel bounds:

$$K_r + \frac{3K_r(K_s - K_r)(1-c)}{3K_r + (K_s - K_r)c} \leq K \leq K_s - \frac{3K_s(K_s - K_r)c}{3K_s + (K_r - K_s)(1-c)} . \tag{3}$$

The hydraulic conductivities of all porous geological media depend strongly on the matric potential. Although the soil component of the mixture will typically be the more conductive at small values of ψ, the rock may in fact become the more permeable component at sufficiently large values of the suction (see Peters and Klavetter, 1988). Hence, a completely general model must be able to allow for arbitrary ratios of K_r/K_s. In the regime of low suctions, at which the conductivity of the rocks is negligible, the Hashin-Shtrikman and the Wiener lower bounds both degenerate to zero. In these cases the Hashin-Shtrikman upper bound is still somewhat more restrictive, and therefore more useful, than the arithmetic mean. Nevertheless, the theoretical bounds only restrict the conductivity to lie within a fairly large range. In order to arrive at more specific predictions of the effective conductivity, we need to consider models that take into account the shape of the rock fragments.

Maxwell-Fricke Model

The effective hydraulic conductivity could in principle be found by solving for the flow through a representative REV that contained a sufficiently large number of rock fragments. It is unfortunately not feasible to solve such problems analytically, and numerical solutions seem to be feasible only for highly idealized geometries (Martinez et al., 1992). Most theoretical approaches to the effective conductivity problem therefore begin by calculating the perturbation in the flowrate caused by a single inclusion in a medium that is subjected to a uniform ''far-field'' potential gradient. This perturbation is then averaged over all possible spatial orientations of the inclusion with respect to the potential gradient. Anisotropic distributions of the inclusion orientations can be accounted for, at the expense of some increase in algebraic complexity

(Artemieva and Chesnokov, 1991; Bachu, 1991). We will only discuss soils in which the orientations of the rock fragments are more or less isotropically distributed. As the analytical results for a single inclusion are strictly applicable only to very small volume fractions, some approximate method must be used to extend the results to higher concentrations. Many such methods have been proposed, but their predictions usually differ substantially only when the volume fraction of the inclusions is greater than about 30%. As the rock fragment volume fractions are not expected to exceed 30% for most soils at Yucca Mountain, we can use one of the simplest of such theories, that developed by Maxwell (1873) and Fricke (1924).

Maxwell (1873) derived the following expression for the effective conductivity K of a medium in which there are dispersed spherical inclusions composed of a second material:

$$\frac{K}{K_s} = \frac{(2+r)-2(1-r)c}{(2+r)+(1-r)c}, \tag{4}$$

where $r = K_r/K_s$ is the ratio of rock conductivity to soil conductivity. In the special case where $K_r = 0$, Maxwell's result reduces to

$$\frac{K}{K_s} = \frac{1-c}{1+0.5c}, \tag{5}$$

which has been used by various authors (Dunn and Mehuys, 1984; Brakensiek et al., 1986b) to account for the effect of inclusions on the saturated hydraulic conductivity of soils. Maxwell's expression coincides with the Hashin-Shtrikman upper bound, as can be seen by rewriting eq. (3) in terms of the conductivity ratio r. Hence, one would expect that angular rock fragments would cause the effective conductivity to lie below Maxwell's result. Dunn and Mehuys (1984) found this to be the case when they measured the saturated conductivities of several Uplands sands that contained up to 20% gravel by volume. They concluded that it would be desirable to have a modification of the Maxwell model that accounted in some way for fragment shape (cf., Peck, 1983).

In order to account for fragment shape, we can use the results of Fricke (1924), who used Maxwell's approach to derive an expression for the effective electrical conductivity of a fluid containing a collection of randomly-oriented spheroids. A spheroid is a degenerate ellipsoid which has two axes of equal length. The shape of a spheroid is characterized by its aspect ratio, α, which is the ratio of the length of the unequal axis to the length of one of the equal axes. Prolate spheroids ($\alpha > 1$) are roughly cigar-shaped, whereas oblate spheroids ($\alpha < 1$) are doorknob-shaped. In its limiting cases, the spheroid can represent a cylindrical fragment ($\alpha \to \infty$), a spherical fragment ($\alpha = 1$), or a thin, disk-like fragment ($\alpha \to 0$). Fricke's expression for the effective conductivity is

$$\frac{K}{K_s} = \frac{(1-c)(1-r) + r\beta c}{(1-c)(1-r) + \beta c}, \tag{6a}$$

$$\beta = \frac{(1-r)}{3}\left[\frac{4}{2+(r-1)M} + \frac{1}{1+(r-1)(1-M)}\right], \tag{6b}$$

where $r = K_r/K_s$, and M is a geometric parameter that for oblate spheroids is given by

$$M = \frac{(2\theta - \sin 2\theta)}{2\tan\theta \sin^2\theta}, \quad \text{where } \theta = \arccos(\alpha), \tag{7}$$

and for prolate spheroids is given by

$$M = \frac{1}{\sin^2\theta} - \frac{\cos^2\theta}{2\sin^3\theta}\ln\left[\frac{1+\sin\theta}{1-\sin\theta}\right], \quad \text{where } \theta = \arccos(1/\alpha). \tag{8}$$

When the inclusions are spherical, $\alpha = 1$ and $M \rightarrow 2/3$, and it can be shown that eq. (6a) reduces to eq. (4). Fricke's expression (6) for the effective conductivity also has the interesting property (Zimmerman, 1989) that the entire range of values permitted by the Hashin-Shtrikman bounds is covered (monotonically) as the aspect ratio varies from 1 to 0. For small inclusion concentrations, $K \approx K_s(1-\beta c)$, so β essentially represents the slope of the curve of normalized conductivity vs. rock volume fraction.

The parameter β is plotted in Fig. 2 for a range of conductivity ratios and aspect ratios. For a fixed aspect ratio, β increases as r decreases, meaning that rock fragments of lower conductivity will cause a more pronounced decrease in the overall conductivity, as would be expected. For a fixed conductivity ratio, β is a minimum for spheres, and approaches asymptotic values in the limiting cases of cylinders or disks. The parameter β is not very sensitive to aspect ratio when $\alpha > 1$, and prolate spheroids therefore have essentially the same effect as spheres. For example, when the fragments are non-conductive, $\beta(\text{spheres}; \alpha = 1) = 1.5$, and $\beta(\text{cylinders}; \alpha = \infty) = 1.67$. Because of this insensitivity, and in light of the fact that rock fragments are more commonly disk-like than cylindrical (Bouwer and Rice, 1984), we will use only oblate spheroids in our modeling. Eq. (6) can also be used in the high-suction regime where we may have $K_r > K_s$, in which case β will be negative. As this regime is of less practical interest, we do not plot curves for $r > 1$ in Fig. 2.

The effective conductivity is plotted in Fig. 3 as a function of rock volume fraction, for various aspect ratios. The conductivity ratio is taken to be 0, although the $r = 0$ curves essentially apply for all $r < 0.01$. For a given volume fraction, spherical fragments cause the minimum decrease in the hydraulic conductivity, whereas flattened disk-like fragments will have the largest effect. Of course, rock fragments will in many cases be somewhat more angular than spheroids. However, there is computational evidence from two-dimensional conductivity problems that the spheroid model can be used to predict effective conductivities, provided that one uses an ''equivalent'' aspect ratio (Zimmerman et al., 1992).

Overall Water Retention Function

Although in many cases the rock fragments may be essentially non-porous, some rock fragments may contain appreciable amounts of water (Coile, 1953; Hanson and Blevins, 1979; Magier and Ravina, 1984). Hence, a general model must account for the water retention properties of both the soil and the rock fragments. In developing our model, we assume again that the rock-filled soil can be treated as a mixture of two porous continua. We therefore ignore any disturbance to the pore structure of the soil that may occur near the interfaces with the rock fragments (cf., Berger, 1976). The water retention function is an equilibrium property, and so a water retention function can be defined for the soil/rock mixture only if the soil and rock fragments are in capillary equilibrium with each other. During transient infiltration processes, this may not always be the case, and it may be more appropriate to model the mixture as a dual-porosity medium (Gerke and van Genuchten, 1993). The characteristic time needed for the mixture to behave as an equivalent porous medium is roughly given by $t^* = \alpha_r \mu \phi_r d_f^2 / k_r$, where α_r is the van Genuchten parameter of the rock material, ϕ_r is its porosity, and $k = \mu K / \rho g$ is its permeability. If the rock is described by, say, a Brooks-Corey water retention function (Brooks and Corey, 1966), then α_r should be replaced by $1/\psi_r^{ae}$, where ψ_r^{ae} is the air-entry pressure of the rock material. The time constant t^* determines the time needed to reach equilibrium during a laboratory measurement of water retention in a soil/rock mixture.

The soil and rock materials are assumed to be governed by two water retention functions, as follows:

$$S_s = F_s(\psi_s), \tag{9a}$$

$$S_r = F_r(\psi_r), \tag{9b}$$

where S is the saturation (volumetric water content θ divided by porosity ϕ), ψ is the matric potential, and F_s and F_r are two arbitrary water retention functions. At equilibrium, the matrix potentials must be equal in the two media, so we can put $\psi_s = \psi_r = \psi$. Now consider a region of the soil/rock mixture that occupies a total volume V, such as in a soil testing apparatus. The soil component occupies a volume $(1-c)V$, which contains a total pore volume $(1-c)V\phi_s$; its water-filled volume will therefore be $(1-c)V\phi_s S_s$. Likewise, the total water-filled volume in the rock fragments is $cV\phi_r S_r$. The total water-filled volume in this region is

$$V_w = (1-c)V\phi_s S_s + cV\phi_r S_r . \tag{10}$$

The mean porosity of this region is

$$\phi = \frac{V_{void}}{V} = \frac{(1-c)V\phi_s + cV\phi_r}{V} = (1-c)\phi_s + c\phi_r . \tag{11}$$

The mean saturation of the region in question is therefore given by

$$S = \frac{V_w}{\phi V} = \frac{(1-c)\phi_s S_s + c\phi_r S_r}{(1-c)\phi_s + c\phi_r} . \tag{12}$$

It is often more convenient to work with the water content, which is given by

$$\theta = \frac{V_w}{V} = (1-c)\phi_s S_s + c\,\phi_r S_r = (1-c)\theta_s + c\,\theta_r\,. \qquad (13)$$

The water content θ_s appearing in eq. (13) denotes the water content that would exist in a soil that contained no rock fragments, measured with respect to the total volume of the soil; similarly for θ_r. The effective water content is therefore given by a simple volumetric average of the water contents of the components. Eq. (13) is equivalent to eq. (10) of Ravina and Magier (1984), except that they define the water content in terms of water volume per unit *weight* of soil, and therefore must include a density term in their equation.

Application of Model to Experimental Data on Hydraulic Conductivity

In order to test the models presented above, it would be necessary to have measurements of hydraulic conductivity and water retention on soils with and without rock fragments. An extensive literature search has unfortunately not revealed many suitable data sets. Two relevant data sets that have been found are the saturated hydraulic conductivity measurements of Dunn and Mehuys (1984), and the water retention measurements of Bouwer and Rice (1984). In the absence of data from soils collected at Yucca Mountain, we will use these two data sets to test our models.

Dunn and Mehuys (1984) performed saturated hydraulic conductivity measurements on a suite of soils that contained varying volume fractions of either spherical glass beads or angular gravel fragments. The soil component of the rock/soil mixtures was in each case an Uplands sand (Typic Haplorthod) with a bulk density of 1.30 g/cm^3, and particle diameters in the range of 0.05–1.0 mm. The length scale of the soils can therefore be taken to be $d_p = 1$ mm. One set of samples were mixed with glass spheres, the diameters of which were 4, 8, 16 or 25 mm. The other set was mixed with angular gravel made from crushed calcareous sandstone and dolomitic limestone. The gravel was sieved to size fractions of 2–5, 5–9, 9–19, or 19–32 mm. Although the rock fragment sizes were always larger than that of the largest soil particles, they did not in all cases satisfy the condition $d_f \gg d_p$, which would be needed to rigorously justify the assumption that the rock/soil system can be treated as a mixture of two continua.

The volume fractions of the inclusions in the various samples were 0.0, 0.025, 0.05, 0.10, and 0.20. The conductivity tests were performed on cylindrical samples having a length of 10 cm and a diameter of 10 cm. For each combination of inclusion type and inclusion size, Dunn and Mehuys (1984) made three conductivity measurements on four nominally identical samples, and then computed the arithmetic mean of the measured values. They also reported the conductivities that were obtained after calculating the geometric mean of the values obtained for the different inclusion sizes. In order to reduce the scatter in the results, and to focus on the effect of the volume fraction and shape of the inclusions, we will analyze this latter set of conductivities that were averaged over the various size fractions. This latter averaging should also tend to mitigate the fact that the rock fragments were not in all cases much larger than the largest soil particles.

Fig. 4 shows the saturated hydraulic conductivity of the soil as a function of the volume fraction of glass spheres. As the inclusions are spherical, we use the original Maxwell equation to model the conductivity, which is equivalent to the Maxwell-Fricke eq. (6) with $\alpha = 1$. If we assume that the rock conductivity is at least two orders of magnitude less than that of the soil, i.e., $r = K_r / K_s < 0.01$, then we can set $r = 0$ in eq. (4), which then leads to eq. (5). Using the measured value of $K_s = 63 \times 10^{-6}$ m/s, we arrive at the prediction that is shown as the solid line in Fig. 4. The predictions are generally reasonably accurate. The maximum discrepancy between the measured and predicted values is 5.8%, and the mean error in the predictions is only 3.1%.

As pointed out by Dunn and Mehuys (1984), their data for the soil that contained the angular rock fragments fell below the predictions of the Maxwell model. We will therefore use the Maxwell-Fricke model for these cases, with an effective aspect ratio that is intended to account for the non-sphericity of the inclusions. No images of the angular gravel are shown in their paper, so it is not possible to estimate the effective aspect ratio *a priori*. Fig. 5 shows the measured average conductivities, along with the predictions of the Maxwell-Fricke model using aspect ratios of 1.0, 0.25, and 0.1. The curve corresponding to an aspect ratio of $\alpha = 0.25$ seems to provide the best fit to the data, yielding a maximum error of 3.9%, and a mean error of 1.6%. Although we cannot compare this value to the actual fragments, an effective aspect ratio of 0.25 does not seem unreasonable for angular rock fragments.

Application of Model to Experimental Data on Water Retention

In order to test the equations presented above for relating the water retention curves with and without large inclusions, we can use the data collected by Bouwer and Rice (1984) on a sand/boulder mixture. Bouwer and Rice (1984) packed a cylindrical container with a mixture of clean cement sand that had a mean particle diameter of $d_p = 0.27$ mm, and Salt River boulders that had an average (equivalent sphere) diameter of $d_f = 12.2$ cm. The volume fraction of boulders was $c = 0.475$. The container had a diameter of 1.24 m, and a height of 2.35 m. This mixture satisfies the criterion that $d_f \gg d_p$. Drainage curves were measured for this sand/boulder mixture, and for the pure sand, over a range of matric potentials from 0 to -10^4 Pa. No measurements were reported for the boulders themselves, but the reported densities of 2.33–2.89 g/cm^3 imply that the boulders were relatively non-porous. As the pores or cracks in the boulders were probably of very small diameter, it is not unreasonable to assume that any water held in the boulders would be immobile over this range of matric potentials. Hence, we can use eq. (13) for these data, without the θ_r term, in the form

$$\theta(\psi, c) = (1-c)\theta_s(\psi). \tag{14}$$

Fig. 6 shows the (drainage) water retention curve for the pure sand, along with the curve for the sand/boulder mixture. The curves are replotted from those shown by Bouwer and Rice (1984), who did not report individual data points. On a log-log plot, eq. (14) predicts that these two curves should be displaced from each other by a factor of $(1-c)=0.525$. For comparison, we have also plotted the curve that is predicted by eq. (14) for the sand/boulder mixture, based on the curve for pure sand. The agreement is reasonably close, although the curves diverge somewhat in the high-suction regime. Note that very long times are required to reach capillary equilibrium in a system whose characteristic length is on the order of one meter, particularly at high suctions where the hydraulic conductivity is low. If the rock/sand mixture did not reach full capillary equilibrium, The fact that the measured water contents were greater than those predicted by eq. (14) could therefore be due to the system not fully attaining capillary equilibrium before the measurements were made.

Conclusions

Two simple models have been presented to account for the presence of rock fragments on the hydrological properties of a soil. The rock/soil mixture is assumed to behave as a mixture of two continua, ignoring any possible surface effects that might be due to disturbance to the soil structure in the vicinity of the rock, for example. The effective water retention curve is essentially given by an appropriate weighted average of the water retention curves for the rock and soil. This model was tested against data reported by Bouwer and Rice (1984) on a sand/boulder mixture, and allowed accurate predictions of the water retention for a sand containing 0.475 volume fraction of boulders, based on data from the same sand without the boulders. A model was proposed for predicting the hydraulic conductivity of a rock/soil mixture based on the assumption that the rock fragments can be treated as oblate spheroids, and then using the Maxwell-Fricke equation. The conductivity model was tested against two data sets on an Uplands sand from Dunn and Mehuys (1984), and again yielded reasonable predictions of the saturated hydraulic conductivity. Thus far, the results of both models seem promising, although the data sets on which they have been tested is limited. In particular, the conductivity model has only been tested for fully-saturated soils. Future work will involve applying these models to data that is currently being collected on unsaturated Yucca Mountain soils by researchers from the U. S. Geological Survey.

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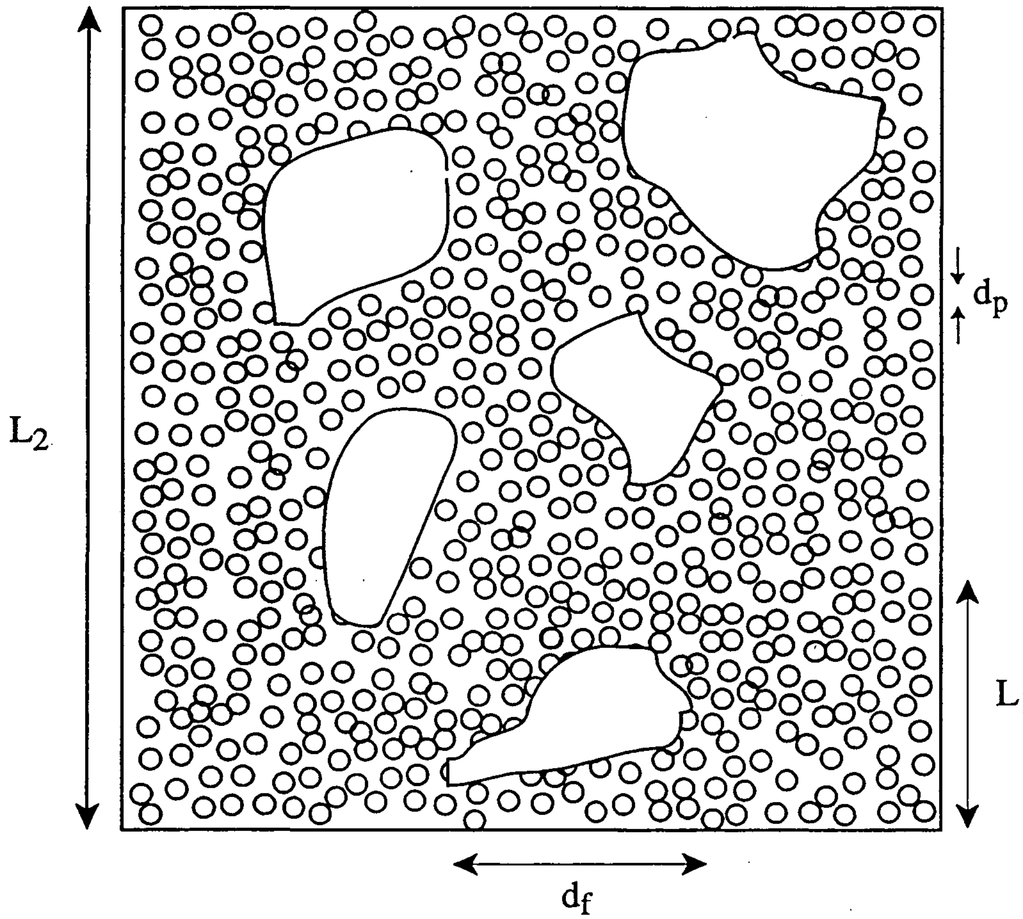

Fig. 1. Schematic diagram of a soil containing rock fragments. The diameter of the largest soil particles is d_p, the REV length of the soil (without fragments) is L_1, the characteristic diameter of the rock fragments is d_f, and the REV scale of the soil/rock mixture is L_2.

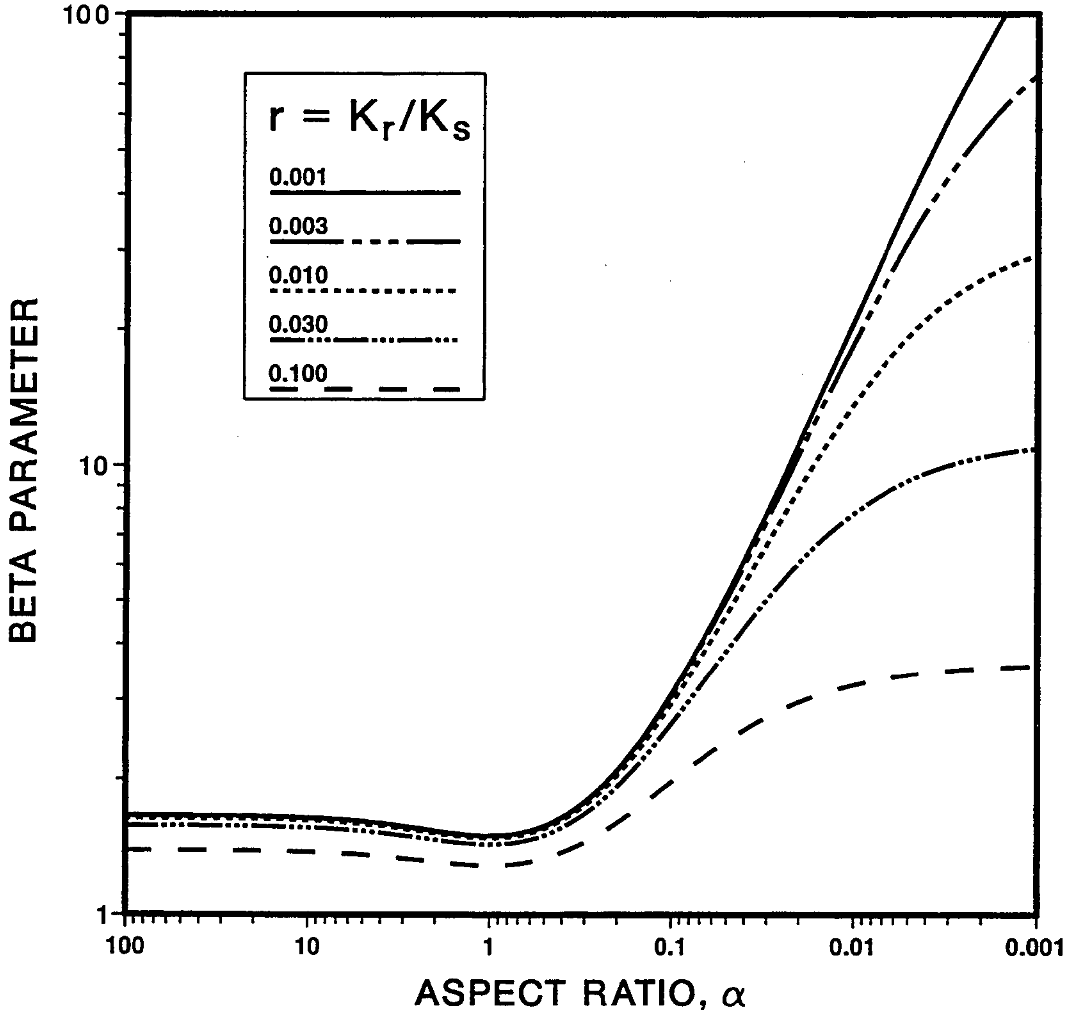

Fig. 2. The parameter β that appears in the Maxwell-Fricke conductivity model, as a function of the aspect ratio of the spheroidal inclusions, for different values of the rock/soil conductivity ratio.

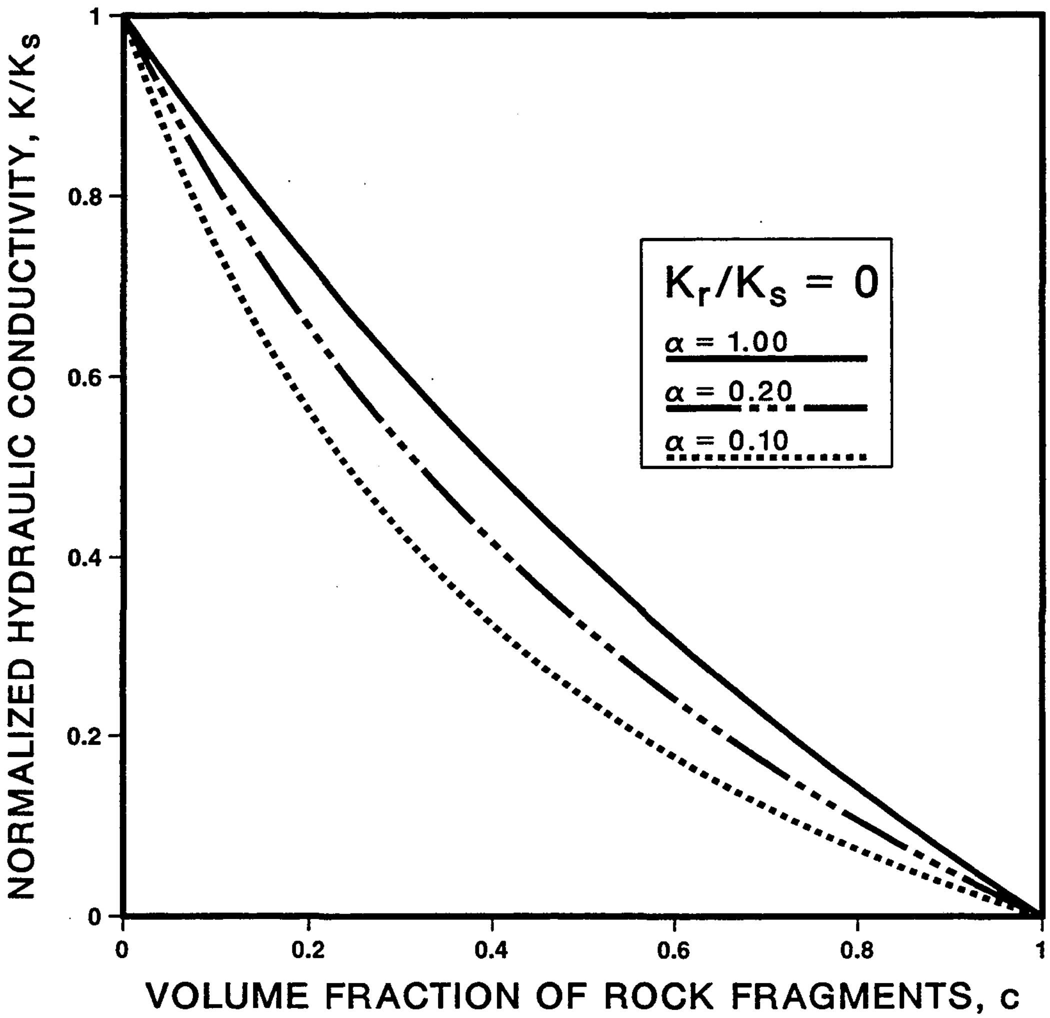

Fig. 3. Normalized effective conductivity predicted by the Maxwell-Fricke conductivity model, as a function of inclusion concentration, for various aspect ratios. The conductivity of the inclusions is taken to be zero.

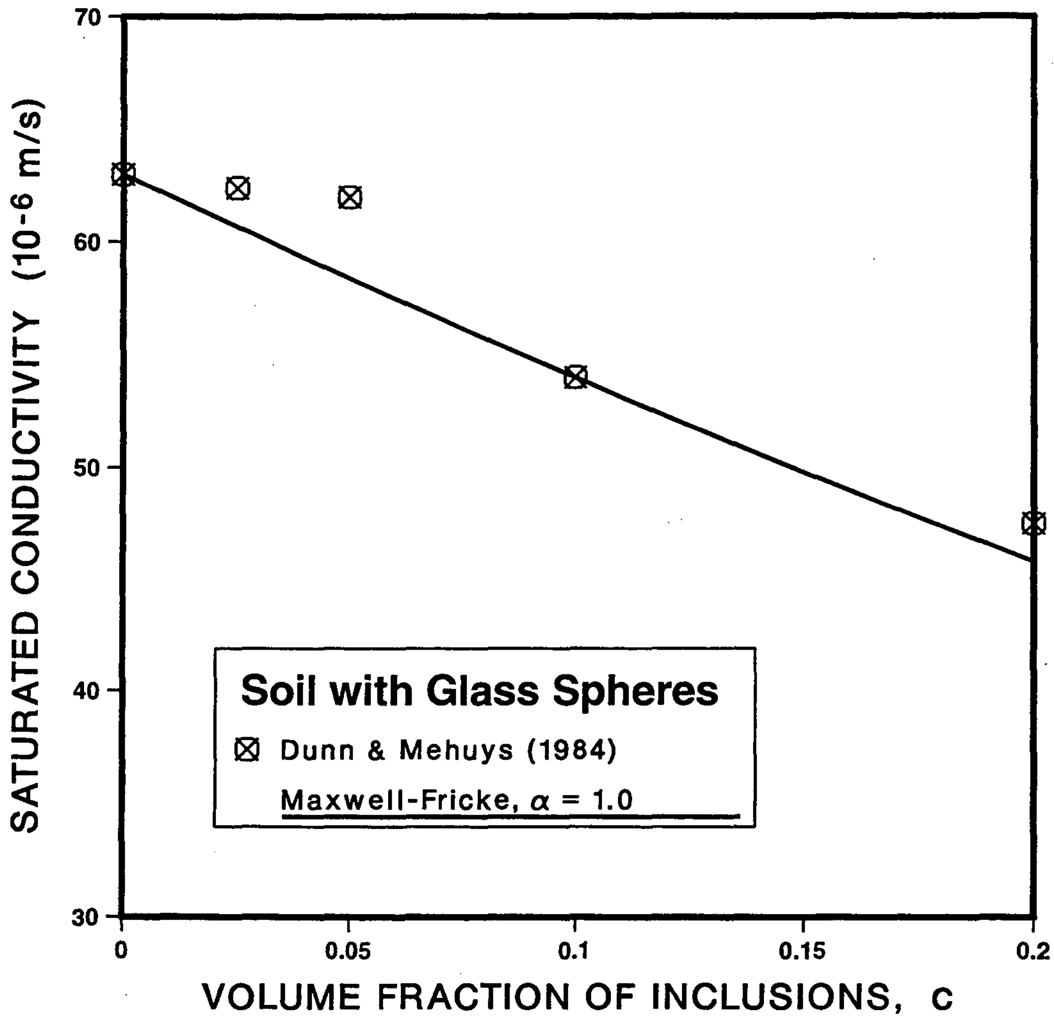

Fig. 4. Hydraulic conductivity of a soil containing spherical glass inclusions. Measured values are from Dunn and Mehuys (1984); predicted values are from eq. (5).

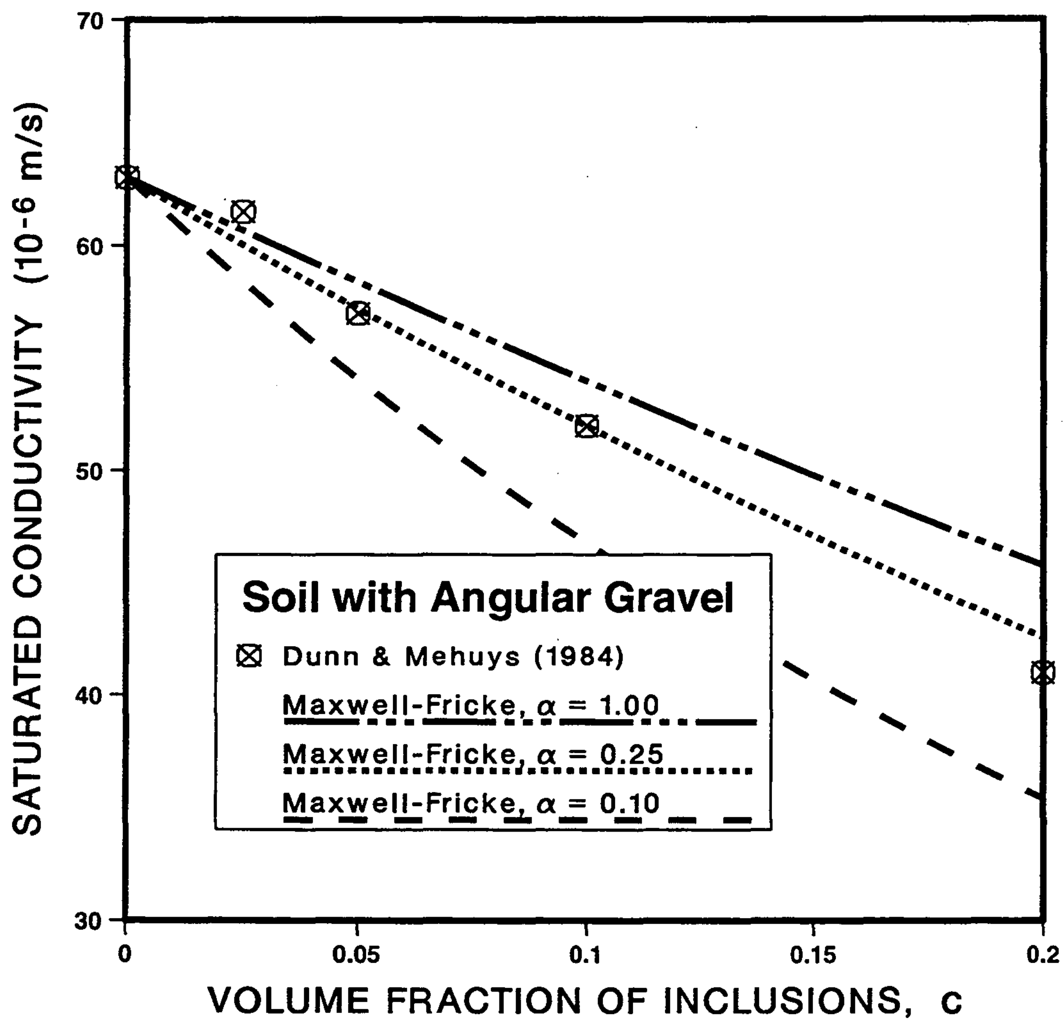

Fig. 5. Hydraulic conductivity of a soil containing angular gravel fragments. Measured values are from Dunn and Mehuys (1984); predicted values are from eq. (6).

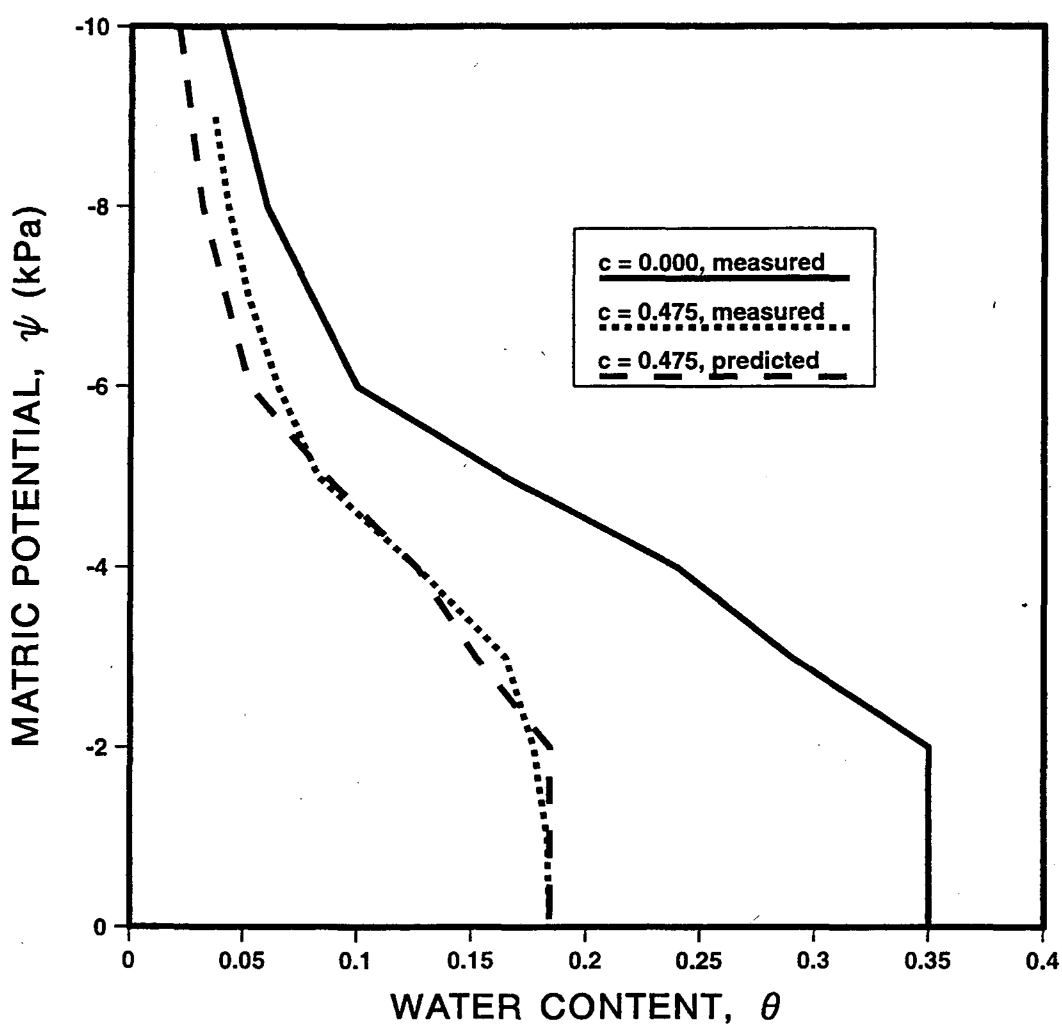

Fig. 6. Water retention (drainage) curves for a sand with volume fractions of 0.0 and 0.475 of boulders. Measured curves are from Bouwer and Rice (1984); predicted curves for $c = 0.475$ are from eq. (14), based on the data for $c = 0.0$.

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