3.6 PERCOLATION THEORETICAL TREATMENTS OF WATER RETENTION AND UNSATURATED HYDRAULIC CONDUCTIVITY: RELEVANCE TO WATER AND ENERGY FLUXES ACROSS THE LAND-AIR INTERFACE

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Accurate prediction of water and energy fluxes across the air/land interface is believed important for climate modeling and for predicting extreme hydrologic events. Thus huge effort has been invested in measurement and classification. But while general understanding of the roles of equilibrium as well as heterogeneity in land surface types and pore-scale constitutive relations is missing, great possibility for internal inconsistency exists. The most poorly understood aspect is that no type of averaging is relevant as a *general* framework for "upscaling" constitutive relations, Hunt, 2001. Though sometimes effects of heterogeneous surfaces may be accounted for by averaging fluxes, this is true for theoretical results only when: 1) linear response holds (i.e. fluxes are linear in a gradient, hysteresis is absent), 2) the gradient is perpendicular to the surface, and 3) the averaging is done at scales above a "representative elementary volume," (the cube of the correlation length in percolation theory). If values are *measured* fluxes, averaging is appropriate iff the measurements are simultaneous. If a three-dimensional problem is considered, transport properties are unrelated to average local values, being given in terms of their values at a percentile, which is typically in the (high permeability) tail of the distribution. The detailed discussion was developed through applying continuum percolation theory to the scaling of the unsaturated to the saturated hydraulic conductivity, $K(S)/K_S$, with S saturation, and then applied to geological heterogeneity up scales, Hunt 2001, 2002a, Hunt and Gee, 2002ab. Side benefits of the investigation were demonstration of the relevance of fractal descriptions of pore space, and their suitability in describing geologic media.

The most important aspect of flow and transport in unsaturated porous media is phase continuity. If K is to be represented as a property of capillary (rather than film, or vapor phase) flow, it must be possible to find a continuous, system spanning path of capillary flow. If there is insufficient liquid water in the medium to maintain a path, then water transport must in some places occur by film flow or vapor phase transport. The minimum moisture content for this condition to be satisfied is called, θ_c, the critical moisture content for percolation. For all $\theta_c<\theta$ K is best found by evaluating critical path analysis, based on percolation theory, Hunt and Gee, 2002b, Bernabe and Bruderer, 1998. In this range of moisture contents $K(S)/K_S$, is found from the ratio of the minimum pore radius that water must flow through at S to its value at full saturation, S=1.

With observations of particle size distributions (PSDs) and the porosity, ϕ, truncated fractal models can be used to calculate the fractal dimensionality, D, of the pore space and thus predict water retention curves of many porous media, Hunt and Gee, 2002b, Filgeuira et al., 1999, Bird et al., 2000. A truncated fractal model is valid for pore sizes between a minimum radius, r_0, and a maximum radius, r_m. The relationship, $\phi=1-(r_0/r_m)^{3-D}$ is obtained, Hunt, 2001, Rieu and Sposito, 1991. For soils in which the PSD exhibits a single slope on a log-log plot, values of D are typically around 2.8. Application of critical path analysis to such a model yields

$$\frac{K(S)}{K_S}=\left[1-\phi\frac{1-S}{1-\theta_c}\right]^{\frac{3}{3-D}} \tag{1}$$

Physical measurements yield D from r_m, r_0 and ϕ,. The only other variables in eqn(1) are $S\equiv\theta/\phi$ and θ_c. But θ_c is the moisture content, at which solute diffusion vanishes, empirically determined (with R^2=0.99) from the surface area to volume ratio of the medium, Moldrup et al., 2001

$$\theta_c = 0.039SA_{vol}^{0.52} \tag{2}$$

Thus eqn(1) for $K(S)$ using θ_c from eqn(2) is a predictive relationship. Values of θ_c range from 3% for coarse sand to 20% for clayey soils. A good approximation for θ_c in sandy soil is $\theta_c\approx\phi/6$, Hunt, 2002b, but the approximation must be modified in clayey soils to account for water films too thin to contribute to capillary flow. Experimental verification of the validity of eqn(1) is thus much more than a fit, it is a verification of the model and the theory as well. Further, it has also been shown that θ_c, given by eqn(2), defines the lower limit of validity of the water retention characteristics derived from fractal media,

$$\theta=\phi-\left[1-\left(\frac{h_A}{h}\right)^{3-D}\right] \tag{3}$$

where h is the hydraulic head, and h_A is its air entry value. It is an important complication that many soils exhibit clearly distinct values of D in different textural ranges, Hunt and Gee, 2002ab; Bittelli et al., 1999; in sandy soils the typical values of D for the sandy part are near 2.8, but for the fine portions, D typically exceeds 2.9. Similarly, in clayey soils, D for the clay may be 2.6, but much larger for the sandy portion. The cause is that D is a diminishing function of the (partial) porosity. A consequence is that increasing D with decreasing pore size (moisture content) in sandy soils tends to steepen $K(h)$ curves relative to those of a simple fractal, with the opposite being the typical condition in clayey soils.

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Sometimes eqns(1) and (3) (and generalizations for more complex media) fail to describe experimental results already for $\theta > \theta_c$. This occurs when $K(S)$ due to capillary flow is so small, that equilibration (i.e. changes in θ with changes in h) do not occur in the time allowed by experiment or nature. The problem of non-equilibrium water retention and hydraulic conductivities has been addressed at the microscopic level, using percolation theory, Hunt, 2002b but a really comprehensive theory is not yet available.

The ratio of the diffusion constant of a solute in porous media, D_{pm}, to its value in water, D_w, is given by, Moldrup et al., 2001

$$\frac{D_{pm}}{D_w} = 1.1\theta\left(\theta - \theta_c\right) \qquad (4)$$

Eqn(4) was derived using percolation theory, closing the circle of interrelated phenomena, Hunt and Ewing, 2002.

It has now been shown that the effective hydraulic conductivity is not a function of scale, Hunt, 2002a. This demonstration was also accomplished using continuum percolation theory (critical path analysis) and a typical critical volume fraction of about 15%. However, the distribution of K values was predicted to narrow from the bottom upwards, both aspects observed in reports of the scale-dependence of the hydraulic conductivity in large basins in the western USA, McPherson et al., 2002.

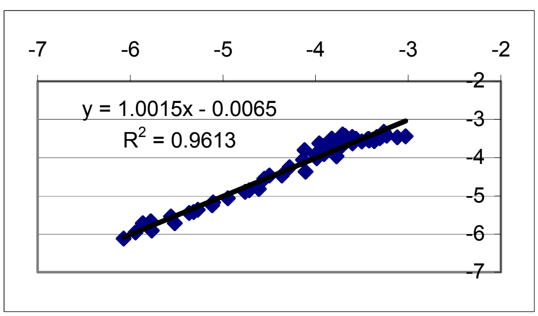

Fig. 1 Measured and predicted values of log[K] for the McGee Ranch Hanford site soil. Experimental values for K are from five depths, while values of D were obtained for 11 samples. Theoretical D values were chosen for individual comparisons with experiment to optimize the agreement under the condition that the mean D as well as its standard deviation, were the same as those obtained from the soil samples. θ_c=0103, was found to optimize the agreement, but the result from the regression on eqn(2) was 0.10, and the optimization was within the limits of the validity of the regression. The mean value of D for those five samples chosen was 2.8302, in comparison with the mean of all 11 of 2.8299, while the corresponding standard deviations were 0.011 and 0.012, respectively.

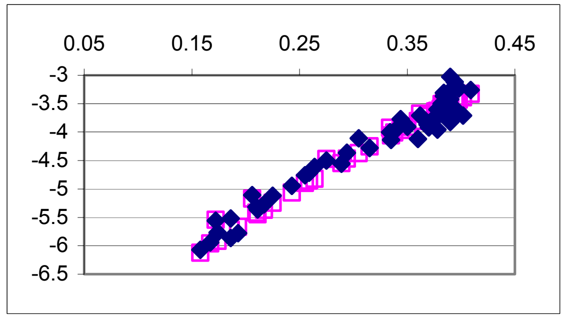

Fig. 2 Experimental values (solid diamonds) of log[K] as a function of θ compared with theory (open squares).

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