Determining Soil Hydraulic Properties from One-step Outflow Experiments by Parameter Estimation: II. Experimental Studies[1]

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ABSTRACT

Unsaturated hydraulic properties of four soils of varying particle size distributions were evaluated by determining values of the five parameters in van Genuchten's (1980) hydraulic model. Saturated conductivities (K_s) and saturated water contents (θ_s) were directly measured and values of residual water content (θ_r) and the parameters α and n were evaluated by a nonlinear inversion method to minimize various objective functions. Method I uses an objective function involving sums of squared deviations between measured cumulative outflow with time $Q(t)$ for one-step pressure desorption and numerically simulated outflow from saturation to a final pressure head $h = -10$ m. Method II supplements $Q(t)$ data with the measured equilibrium water content θ at $h = -150$ m, while Method III employs equilibrium $\theta(h)$ data only. Method I yields the most accurate description of $Q(t)$ and the independently determined hydraulic diffusivity $D(\theta)$. A fair description of $\theta(h)$ is obtained within the range of the one-step experiment but at lower θ predictions are less reliable especially for finer-textured soil. Method II extends the range of validity of the predicted $\theta(h)$ to lower θ with generally small effects on predicted $D(\theta)$ and $Q(t)$. Method III gives the best description of $\theta(h)$ but at the expense of accuracy in $Q(t)$ and $D(\theta)$. Implications for routine evaluation of soil hydraulic properties are discussed.

Additional Index Words: **unsaturated hydraulic conductivity measurement, water retention measurement, soil water diffusivity, inverse problem, optimization.**

Parker, J.C., J.B. Kool, and M.Th. van Genuchten. 1985. Determining soil hydraulic properties from one-step outflow experiments by parameter estimation: II. Experimental studies. Soil Sci. Soc. Am. J. 49:1354–1359.

THE PARAMETER estimation approach to determining soil hydraulic properties from transient flow experiments is based on the premise that assumed expressions for the soil hydraulic properties accurately describe the real system and that the inversion problem has a unique solution. In Part I of this paper (Kool et al., 1985a), we found that to minimize uniqueness problems, transient flow data used as input to an inversion procedure should correspond to as broad a range in soil water contents as possible. For gravity drainage experiments, such as those considered by Zachman et al. (1981, 1982) and Hornung (1983), the minimum pressure head obtained depends directly on the height of the soil column. For reasonably attainable laboratory column lengths, ranges in water content will accordingly be very narrow for all but the coarsest textured soils, thus severely limiting the practical applicability of such procedures based on gravity drainage only.

Dane and Hruska (1983) applied parameter estimation methods to the determination of in situ hydraulic properties using input data consisting of water content profiles at different times during gravity drainage of a clay loam soil with a zero flux condition at the soil surface. Good results were obtained; however, as with the laboratory gravity drainage experiments, limitations occurred on the attainable range in water contents and experiment durations had to be rather long. In their case, observations were extended to 25 d.

Pressure desorption of short soil cores offers an experimentally simple method of obtaining data for parameter estimation suitable to a broad range of soils. In Part I we investigated numerical constraints on the feasibility of estimating hydraulic properties by inversion of cumulative pressure outflow data measured with time from short soil cores. Van Genuchten's (1978, 1980) hydraulic property model was employed with two of the five model parameters assumed independently measured and three estimated by numerical inversion. This approach was shown to be feasible provided: (i) the pressure increment is large enough to yield a low final reduced water content, (ii) outflow measurements are extended over an adequate period of time, (iii) initial parameter estimates are reasonably close to their true values, and (iv) experimental error is relatively small. Additionally, the success of this method will depend on whether the assumed model accurately describes soil hydraulic properties.

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Table 1. Characterization of soils studied.

Textural class	Particle size distribution Sand	Silt	Clay	Bulk density	Description
	%			kg m^{-3}	
Sandy loam	61	24	15	1550	A horizon, granular structure
Silt loam	28	56	15	1570	A horizon, granular structure
Sandy clay loam	56	18	26	1530	A horizon, granular structure
Clay	21	31	48	1110	C horizon, massive weathered shale

Table 2. Measured values of saturated water contents (θ_s), saturated conductivities of soil cores (K_s), and of ceramic plates (K_p) used in inverse problem solutions.

Soil	θ_s	K_s	K_p
	m^3 m^{-3}	m s^{-1}	
Sandy loam	0.355	7.0×10^{-7}	5.5×10^{-9}
Silt loam	0.388	1.5×10^{-5}	8.3×10^{-9}
Sandy clay loam	0.402	1.1×10^{-6}	5.5×10^{-9}
Clay	0.589	2.2×10^{-9}	1.4×10^{-8}

Table 3. Parameter values for van Genuchten model determined from transient one-step outflow experiments.

Soil	Parameter	Initial values†	Final parameter values† Method I	Method II	Method III
Sandy loam	α	2.50	1.29	1.23	1.53
	n	1.50	1.511	1.301	1.265
	θ_r	0.15	0.183	0.110	0.074
Silt loam	α	2.50	3.35	4.71	3.46
	n	1.50	1.387	1.461	1.289
	θ_r	0.20	0.161	0.173	0.103
Sandy clay loam	α	1.00	2.15	2.34	0.82
	n	1.50	1.217	1.225	1.275
	θ_r	0.30	0.200	0.199	0.112
Clay	α	0.50	0.15	0.08	0.07
	n	1.50	1.485	1.319	1.419
	θ_r	0.40	0.395	0.127	0.109

† Units of α in m^{-1}, θ_r in m^3 m^{-3}, n dimensionless.

Zachman et al. (1982) have shown that when an incorrect model for the soil hydraulic properties is used, it may still be possible to obtain an apparently acceptable solution to the inversion problem; however, the hydraulic functions corresponding to the solution may be in error.

In the present paper, we investigate effects of experimental variables and model accuracy on hydraulic property estimation from one-step pressure outflow experiments on undisturbed soil cores.

METHODS AND MATERIALS

Single undisturbed soil cores of 54-mm diam and 40-mm length were taken from four locations with a thin-wall hydraulic core sampler for laboratory testing. The soil texture ranged from sandy loam to clay (Table 1). Cores were assembled in Tempe pressure cells with 5.7-mm thick, -10 m air-entry ceramic plates. To ensure reproducibility of the main drying curves, cores were preconditioned by subjecting them to several wetting and drying cycles between pressure heads of 0 and -10 m. Final saturation was accomplished by wetting the cores from the bottom at a pressure head of -0.1 m, followed after equilibration by gradually increasing the head to $h = 0$ at the top of the core. A 0.01 M $CaCl_2$ solution was used in all experiments to minimize soil dispersion.

One-step pressure outflow tests were performed for a pneumatic head increment h^a of 10 m at the top of the cores. Cumulative outflow volume was measured as a function of time with a burette arranged to allow adjustment of the outflow free surface to the midheight of the core and to permit flushing of trapped air from beneath the porous plate. Due to small but measureable evaporative losses from connecting tubing, "blank" cells were monitored to allow appropriate corrections to be made on outflow measurements. Further details of the experimental apparatus and techniques are given by Kool et al. (1985b).

After resaturating the cores in the same manner as before, stepwise desorption experiments were carried out to determine the equilibrium water retention characteristics. Equilibrium outflow volumes were measured as the cores were desorbed incrementally to pressure heads of -0.1, -0.5, -1.0, -3.0, -6.0, and -10.0 m. After resaturating the soil and again desorbing to -0.1 m, the cores were removed from the cells and weighed to permit subsequent gravimetric determination of the $h = -0.1$-m water content used as a reference point for calculation of other equilibrium water contents from outflow measurements. Oven-dry core masses were obtained after determining saturated hydraulic conductivities of the cores (K_s) by a falling-head method. The porous plates were for that purpose replaced by low impedance filters. Hydraulic conductivities of the porous ceramic plates (K_p) were determined in a similar fashion.

Volumetric water contents θ at pressure heads of -30 and -150 m were determined on air-dried and sieved samples of the four soils by pressure desorption using undisturbed core densities to convert from gravimetric to volumetric water contents.

RESULTS AND DISCUSSION

We used the cumulative outflow data with time to calculate the van Genuchten model parameters by numerical inversion of the flow problem as outlined in Part I. Measured values of θ_s, K_s, and K_p (Table 2) were input as knowns and unconstrained values of the parameters α, n, and θ_r were obtained by inversion from initial values judged appropriate for the respective sample particle size distributions. Initial parameter values and final fitted values obtained in this manner, denoted as Method I, are given in Table 3. All inversion problems were run at least twice with different initial parameter estimates. In cases where solutions did not converge to the same final estimates, the estimates that led to the highest r^2 values are reported. For the cases shown in the table, convergence to final values was obtained within 28 to 39 trial solutions.

Comparison of observed and fitted cumulative outflow data (Fig. 1, Method I) indicates that reasonably accurate flow predictions are obtained. Because the objective function for inversion utilizes outflow data, we must turn to independent measurements of hydraulic behavior for corroboration of the model. First, we compared the transient outflow-derived $\theta(h)$-curve with conventionally measured static stepwise desorption data. As seen in Fig. 2, reasonable correspondence is obtained between measured equilibrium $\theta(h)$ and the transient (Method I) derived functions over the range of h from 0 to -10 m obtained during the one-step outflow experiments. For lower h, predicted and directly measured $\theta(h)$ tend to diverge increasingly,

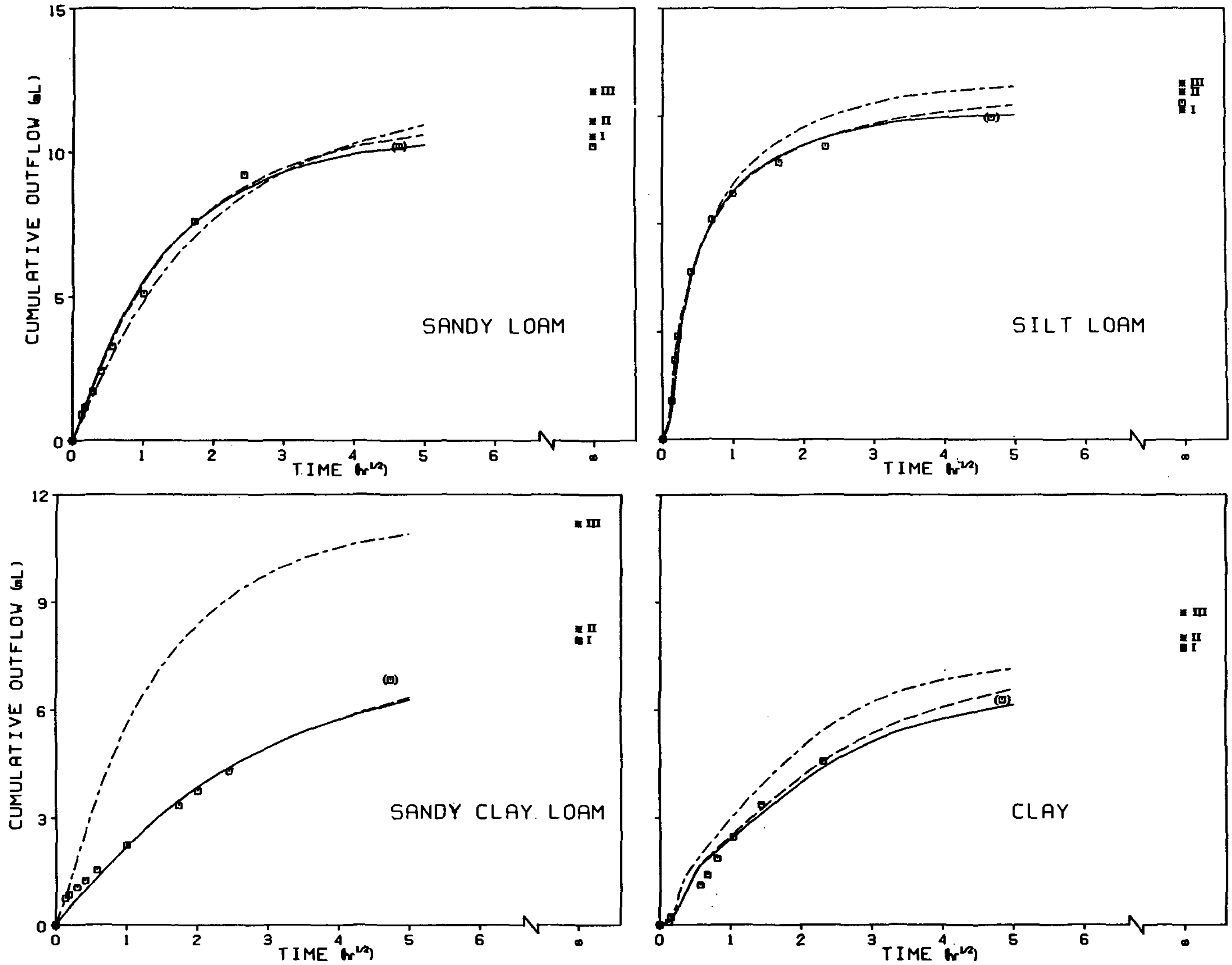

Fig. 1. Measured cumulative outflow from soil cores (□ datapoints) and predicted outflow using hydraulic properties evaluated by parameter estimation from outflow data only (———: Method I), from outflow data supplemented by the measured θ at h = −150 m (—— ——: Method II), and from measured θ (h) data only (—— – – ——: Method III). Data points in parentheses werenot used in inversion procedure. * indicates $\hat{Q}(t_\infty)$.

particularly for the finer textured soils. These soils exhibit narrower ranges in water contents over the imposed pressure head range, possibly resulting in nonunique inversion results. Such difficulties could be reduced by using larger gas pressure increments for finer textured soils. Conversely, we note that for very coarse textured soil, a smaller pressure increment may be necessary to obtain adequate resolution in outflow-time data to permit inversion.

Another approach to reducing prediction errors at low potentials is to incorporate selected measured $\theta(h)$-data into the objective function which is to be minimized as:

$$E(b) = \sum_{i=1}^{N} \{w_i[\,Q(t_i) - \hat{Q}(t_i,b)]\}^2 + \sum_{j=1}^{M} \{v_j[\theta(h_j) - \hat{\theta}(h_j,b)]\}^2 \qquad [1]$$

where b is the vector of parameter estimates, Q and $\hat{Q}$ are observed and predicted transient outflow volumes, θ and $\hat{\theta}$ are observed and predicted water contents at specified h, and w_i and v_j are weighting factors. Evaluation of $\hat{\theta}$ is obtained directly via Eq. [4] of Part I. In our modified parameter estimation approach, we employ the same $Q(t)$ data as before with $w_i = 1$ and include one (θ, h_j) pair for $h = -150$ m (M = 1). To give $\theta(h)$ values approximately the same weight as $Q(t)$ values we take

$$v_j = M \sum_{i=1}^{N} Q(t_i) \Big/ N \sum_{j=1}^{M} \theta(h_j) \qquad [2]$$

Parameter values from this modified method, denoted as Method II, are given in Table 3. For the sandy loam and clay soils, Method II results in better correspondence between observed and predicted θ(h) for $h \leq -10$ m (Fig. 2). Except perhaps for the silt loam, there is little change in the range $-10 < h < 0$. Correspondence between observed and calculated out-

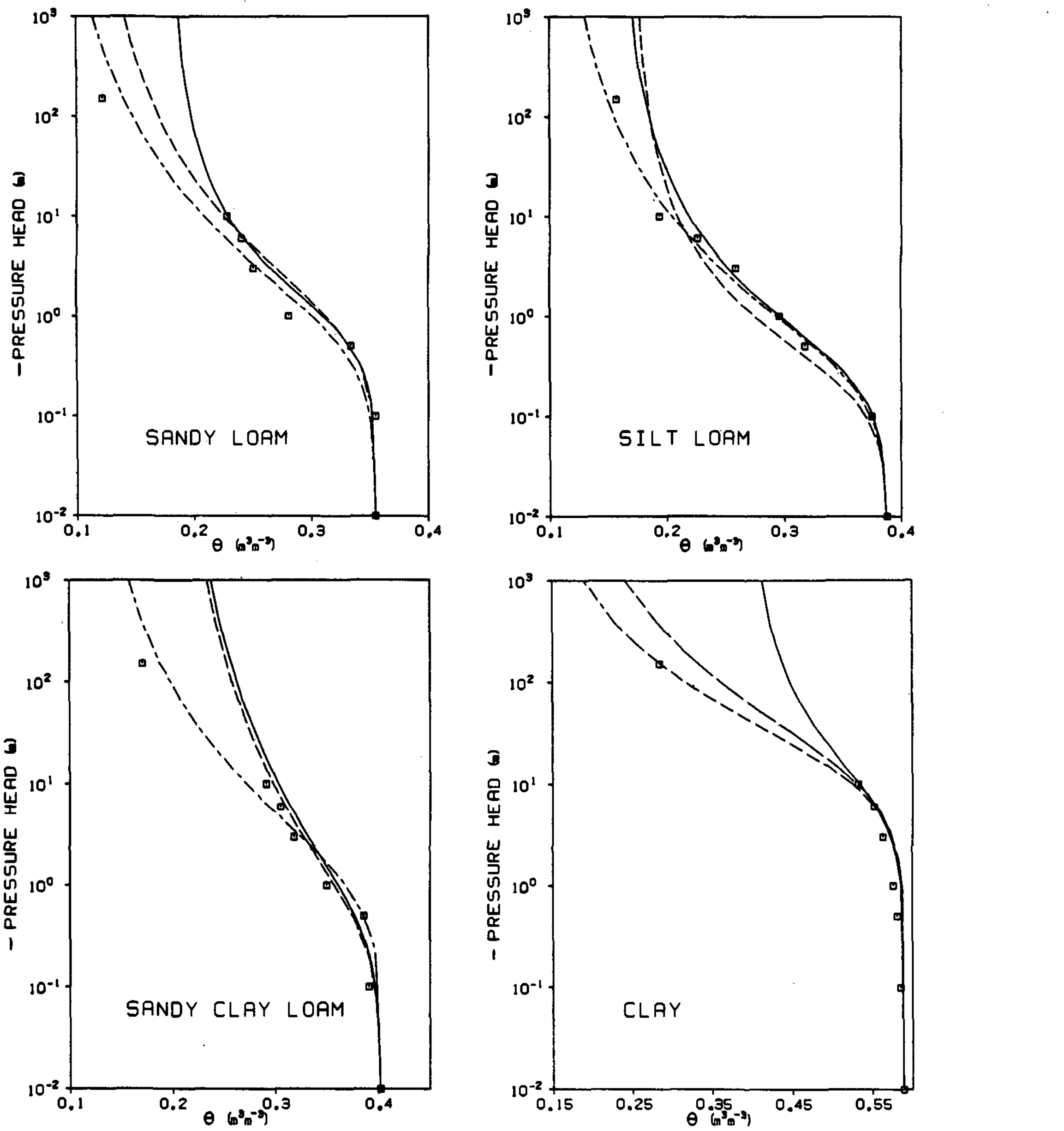

Fig. 2. Measured θ(*h*) by static stepwise desorption (datapoints) and predicted θ(*h*) from parameter values evaluated by Methods I, II, and III. ———: Method I, — — —: Method II, — - —: Method III.

flow (Fig. 1) is likewise not greatly affected by the additional constraint imposed on the inverse problem.

Besides experimental errors in observed *Q(t)* and θ(*h*), discrepancies between observed θ(*h*) and those predicted by Methods I and II may be due to nonuniqueness of the inverse problems or to deviations of actual hydraulic properties from the assumed parametric model. To investigate this we carried out the parameter estimation process using only measured equilibrium θ(*h*) for $h = 0$ to -150 m in the objective function with no transient flow data ($N = 0$). Parameter values from this method, denoted Method III (Table 3), yield θ(*h*)-curves which more closely match directly measured θ(*h*) data than the curves derived from the transient outflow measurements (Fig. 2). Comparison of the calculated outflow-time curves in Fig. 1 shows that for three of the four soils, Method III gives predictions of the transient hydraulic behavior that are the same or reasonably similar to the calculations obtained with Methods I and II. However, the predicted outflow curve (Method III) for the sandy clay loam soil is significantly higher than the observed or directly fitted curves I and II. This suggests that, at least for this soil, differences in parameter values obtained by Method III vs. those by Methods I or II should be partially attributed to deviations from the assumed parametric model for the hydraulic properties and not merely to nonuniqueness of the inverse problem.

The accuracy of the hydraulic model and the appropriateness of the various parameter estimation schemes may be further evaluated by comparison of hydraulic diffusivities ($D = Kdh/d\theta$) predicted from parameters estimated by Methods I through III and those calculated directly from one-step outflow data using the method of Passioura (1976). In this proce-

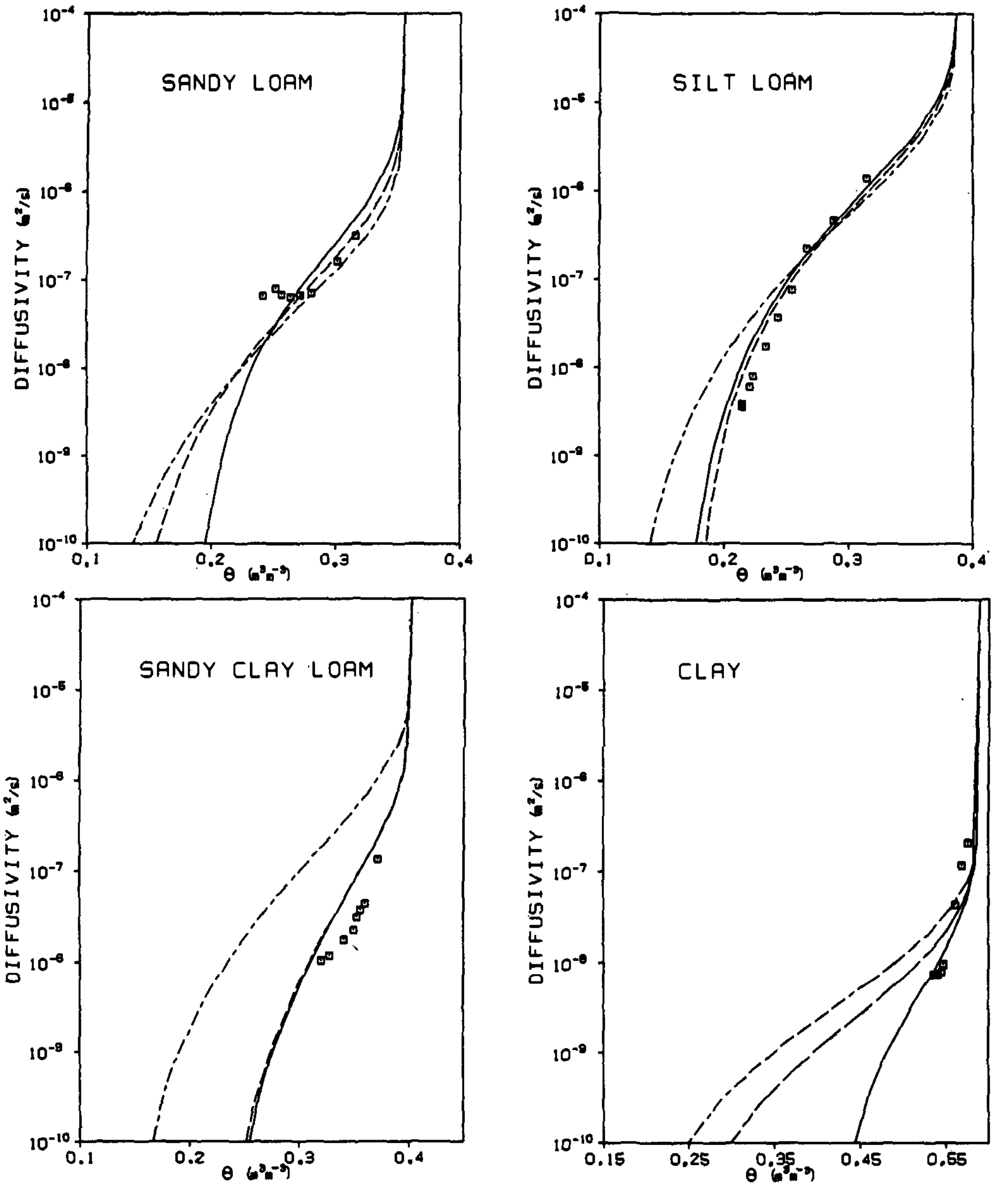

Fig. 3. Calculated $D(\theta)$ by method of Passioura, 1976 (datapoints) and predicted $D(\theta)$ from parameter values evaluated by Methods I, II, and III. ———: Method I, —— ——: Method II, —— – ——: Method III.

dure, the first part of the outflow vs. time curve is not used. Hence, diffusivities are obtained only for a narrow range of moisture contents. Passioura's method calculates $D(\theta)$ from the ratio of second derivative to first derivative of the outflow vs. time curve. The procedure is therefore not very accurate when θ approaches its equilibrium value as both the numerator and denominator tend to zero. This could explain the aberrant behavior of the calculated $D(\theta)$ for $\theta < 0.275$ for the sandy loam. Keeping in mind the approximate nature of the calculated $D(\theta)$ when comparing these with predicted $D(\theta)$-curves (Fig. 3), correspondence between the predictions of Methods I and II and Passioura's results is judged to be excellent while for Method III the results are poorer. Only the sandy clay loam soil shows an unacceptable prediction of $D(\theta)$ with Method III. Figure 3 also shows that predicted $D(\theta)$-curves diverge as θ decreases, again reflecting the differences in fitted θ_r values.

SUMMARY AND CONCLUSIONS

Because of experimental difficulties involved in the "direct" measurement of unsaturated hydraulic conductivities (i.e., from data amenable to analytic solution of the inverse problem), the most appealing method of evaluating unsaturated soil properties is by application of pore structure models which yield $K(h)$ from equilibrium $\theta(h)$-data and the saturated conductivity. The use of parametric formulations for $\theta(h)$ which lead to closed-form expressions for $K(h)$ and $C(h) = d\theta/dh$, represents a very convenient method of characterizing soil hydraulic behavior. Here we employ van Genuchten's hydraulic model, chosen because it is simple and yet has been found to describe with reasonable accuracy the hydraulic properties of a variety of soils.

The most common method of estimating parameters in this and similar models is by best-fitting to equilibrium $\theta(h)$-data only. When deviations between measured and predicted $\theta(h)$ are used to formulate an objective function for parameter estimation, any inaccuracies in the hydraulic model will be forced into the predicted $K(h)$. An alternative approach using transient flow data to formulate the objective function will distribute errors due to model inaccuracies to both $\theta(h)$ and $K(h)$ in a manner which optimizes the ability of the model to describe the entire transient flow process.

We have compared three types of sums-of-squared deviations objective functions for parameter estimation using observed data consisting of (Method I) cumulative outflow with time from initial saturation following a one-step pneumatic head increment of 10 m, (Method II) cumulative outflow data supplemented by the measured water content at $h = -150$ m, and (Method III) equilibrium $\theta(h)$ data only without transient flow measurements. Method I yields satisfactory results within the range of water contents observed in the transient experiment but cannot be reliably extrapolated to lower θ especially for fine-textured soils. Method II extends the range of validity of predicted properties to low θ with only minor effects on the predictions at high θ. Method III yields a more accurate description of $\theta(h)$ than Methods I and II but sometimes at the expense of accuracy in $K(h)$ and in predictions of transient flow, thus reflecting the biases inherent in the various objective functions employed.

Since the purpose of hydraulic property estimation is ultimately to enable accurate predictions of flow behavior, and also considering the tendency toward widespread use of approximate pore structure models, employing transient flow data rather than equilibrium $\theta(h)$ may be more appropriate for the estimation of soil hydraulic properties. Because one-step outflow tests can be performed in much less time than stepwise equilibrium desorption tests, use of the former is especially attractive when intensive field-sampling of soil hydraulic properties is needed for validation or implementation of stochastic flow models.

In this paper we have investigated the numerical inversion of laboratory pressure outflow data to yield information on hydraulic behavior during monotonic drying. To more accurately predict transient hydraulic behavior, it will be necessary to also consider wetting phenomena owing to hysteresis in soil hydraulic properties. Extension of the parameter estimation approach involving solution of the inverse flow problem to the analysis of inflow experiments to characterize hysteretic behavior is currently being investigated. As with all laboratory analyses, care must be exercised to ensure that sample disturbance does not inordinately effect the results. In subsequent work the extension of parameter estimation methods to in situ experiments will be investigated.

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