Determining Soil Hydraulic Properties from One-step Outflow Experiments by Parameter Estimation: I. Theory and Numerical Studies[1]

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ABSTRACT

The numerical feasibility of determining water retention and hydraulic conductivity functions simultaneously from one-step pressure outflow experiments on soil cores by a parameter estimation method is evaluated. Soil hydraulic properties are assumed to be represented by van Genuchten's closed-form expressions involving three unknown parameters: residual moisture content θ_r and coefficients α and n. These parameters are evaluated by nonlinear least-squares fitting of predicted to observed cumulative outflow with time. Numerical experiments were performed for two hypothetical soils to evaluate limitations of the method imposed by constraints of uniqueness and sensitivity to error. Results indicate that an accurate solution of the parameter identification problem may be obtained when (i) input data include cumulative outflow volumes with time corresponding to at least half of the final outflow and additionally the final outflow volume; (ii) final cumulative outflow corresponds to a sufficiently large fraction (e.g., >0.5) of the total water between saturated and residual water contents; (iii) experimental error in outflow measurements is low; and (iv) initial parameter estimates are reasonably close to their true values.

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

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THE INCREASING REALIZATION that knowledge of spatial variability of soil hydraulic properties is of paramount importance for the prediction of field-scale flow and transport processes has greatly accentuated the need for more efficient means of determining these properties. Recently, interest has arisen in the feasibility of simultaneously determining water retention and hydraulic conductivity functions from transient flow data by parameter estimation methods (Zachman et al., 1981; 1982; Dane and Hruska, 1983; Hornung, 1983). Since transient flow data can be relatively quickly obtained, much of the tedious and time consuming nature of more conventional methods of determining hydraulic properties may be avoided. The parameter estimation approach is based on the assumption that relationships between volumetric water content θ, hydraulic conductivity K, and pressure head h are described by known mathematical expressions with a small number of parameters. (In this paper we use the term *pressure head* to refer to the components of total potential attributable to matric and hydrostatic components but excluding nonatmospheric gas pressure contributions.) The problem of determining $\theta(h)$ and $K(h)$ thus becomes a problem of determining values of the initially unknown parameters. Experimentally, the procedures involve measurement of some flux-controlled attribute(s) during transient flow. The flow process is then simulated numerically using guessed initial values of the unknown parameters. Simulations are repeated with improved parameter estimates until simulated and observed results match.

Assuming that sufficiently accurate expressions for $\theta(h)$ and $K(h)$ are used, the main requirement for the parameter estimation problem is that the input data contain sufficient information to define a unique solution. Hornung (1983) considered a hypothetical experiment in which a vertical column, initially at hydrostatic equilibrium with zero matric potential at the lower boundary is subjected to a constant downward flux at the upper surface. Two unknown parameters in a five parameter model for the soil hydraulic prop-

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erties were determined from column outflow rates. It was concluded that under these experimental conditions outflow rates alone do not give sufficient information to satisfy uniqueness. Only when additional information was included in the input data could the uniqueness problem be resolved. Hornung used the final steady state pressure head at a fixed point inside the column as additional input. Zachman et al. (1981) considered a similar problem involving gravity drainage from an initially saturated column of sand and investigated the usefulness of various types of measurements for estimating the coefficients in a four parameter model with two coefficients assumed known. They concluded that cumulative drainage vs. time yielded the best results while offering the additional advantage that the data are easily obtained. No problems involving uniqueness were reported.

We wish to investigate the feasibility of using a parameter estimation approach to obtain $\theta(h)$ and $K(h)$ from measurements of cumulative outflow with time from initially saturated soil in a pressure desorption cell following a step change in gas pressure. Experimental details and results for undisturbed soil cores will be presented in a companion paper (Parker et al., 1985). Here, we present the theoretical background of the method and investigate numerical constraints of the technique by evaluating solution uniqueness and sensitivity to errors in input data for two hypothetical soils.

THEORY

Hydraulic Model

The experimental procedure which we consider involves the measurement of cumulative outflow with time from a soil core at high initial water content, subjected to an instantaneous increment in pneumatic pressure at the top with a saturated porous plate in place at the bottom. We require a solution of Richards' equation which may be written for the one-dimensional case with vertical distance x taken positive downward and with pneumatic potentials translated to the lower boundary condition for notational convenience:

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}[K(h)(\partial h/\partial x - 1)] \qquad [1]$$

where $C = d\theta/dh$ is the water capacity. The appropriate initial and boundary conditions are

$$h = h_o(x) \qquad t = 0, \quad 0 \leq x \leq L \qquad [2a]$$

$$\partial h/\partial x = 1 \qquad t > 0, \quad x = 0 \qquad [2b]$$

$$h = h_L - h^a \qquad t > 0, \quad x = L \qquad [2c]$$

where $x = 0$ is taken at the top of the core, $x = L$ is the bottom of the porous plate, h_L is the pressure head at the bottom of the porous plate, and $h_a = \Delta p/\rho g$ where Δp is the gauge gas pressure applied to the core, g is gravitational acceleration, and ρ is the density of water. For the problem under consideration, we solve Eq. [1] for the two-layer system of soil column and porous plate. Since the porous plate remains saturated, hydraulic properties of the plate in the pressure cell will be independent of h with $C = 0$ and $K = K_p$.

The solution of Eq. [1] and [2] was obtained by a modified version of the Galerkin finite element model of van Genuchten (1978b). Cumulative outflow $Q(t)$ was subsequently calculated as

$$Q(t) = A\int_0^L [\theta(x,0) - \theta(x,t)]\, dx \qquad [3]$$

where A is the core area perpendicular to flow. The integral in Eq. [3] is evaluated using the composite trapezoidal rule.

We assume soil hydraulic properties are described by van Genuchten's model (van Genuchten, 1978a; 1980):

$$\Theta = \begin{cases} \dfrac{1}{[1 + |\alpha h|^n]^{1-1/n}} & h < 0 \\ 1 & h \geq 0 \end{cases} \qquad [4]$$

$$K = K_s\Theta^{1/2}\left[1 - (1 - \Theta^{n/(n-1)})^{1-1/n}\right]^2 \qquad (n > 1) \qquad [5]$$

and

$$\Theta = (\theta - \theta_r)/(\theta_s - \theta_r) \qquad [6]$$

where θ_s is the saturated water content (θ at $h = 0$); θ_r is the "residual" water content; K_s is the saturated hydraulic conductivity; and α and n are empirical parameters. Expressions for $K(h)$ and $C(h)$ follow from Eq. [4] through [6]. Of the five parameters K_s, θ_s, θ_r, α, and n in these expressions, the first two have clear physical significance. The residual water content is defined nominally as the water content at which $K \rightarrow 0$ and $h \rightarrow -\infty$. Literally, this condition is only met if $\theta_r = 0$. In practice, Eq. [4] through [6] are not applied at very low pressure heads (e.g., $h < -150$m) and θ_r must be regarded as a strictly empirical coefficient which yields the best fit to the data over the desired range in θ. The parameters α and n are inversely related to the air-entry tension and width of the pore size distribution, respectively (van Genuchten, 1978a). From our own data and that in the literature, we observe that for desorption, α generally ranges from 0.5 to 5.0 m^{-1}, while n usually varies from 1.1 to about 3.5 (van Genuchten, 1980; van Genuchten and Nielsen, 1985). For α, the lowest value reported is 0.15 m^{-1} for a heavy clay soil, while for n the upper limit is about 10 for materials with extremely narrow pore size distributions. High values of α and n generally correspond to sandy soils while fine-textured soils have lower values.

In the parameter estimation problem we assume that θ_s, K_s, and K_p have been measured independently. Values of θ_r, α, and n are sought by numerical inversion of the flow problem.

Parameter Estimation Procedure

The experimental procedure results in a set of cumulative outflow measurements Q at specific times t_i ($i = 1,2,\ldots N$). These $Q(t_i)$ are employed as input data for the numerical inversion problem. Let $\hat{Q}(b,t_i)$ be the numerically calculated values of outflow corresponding to a trial vector of parameter values $\{b\}$ where $\{b\}$ is the three-dimensional vector $\{\alpha, n, \theta_r\}$. The problem we pose is to find an optimum combination of parameters $\{b°\}$ that minimizes the objective function:

$$E(b) = \sum_{i=1}^{N}\left\{w_i[\,Q(t_i) - \hat{Q}(t_i, b)]\right\}^2 \qquad [8]$$

where w_i is a weighting function taken as unity in the simulations considered here. To determine $\{b°\}$ we employ an optimization algorithm based on Marquardt's maximum neighborhood method (Marquardt, 1963). This method represents an optimum combination of the method of steepest descent and the Gauss-Newton method, and is widely used for nonlinear least-squares optimization (Beck and Arnold, 1977).

We wish to investigate the adequacy of cumulative outflow volumes $[Q(t_1),\ldots Q(t_N)]$ observed at times $t_1,\ldots,t_N$ to define unique solutions to the inverse problem. It is antic-

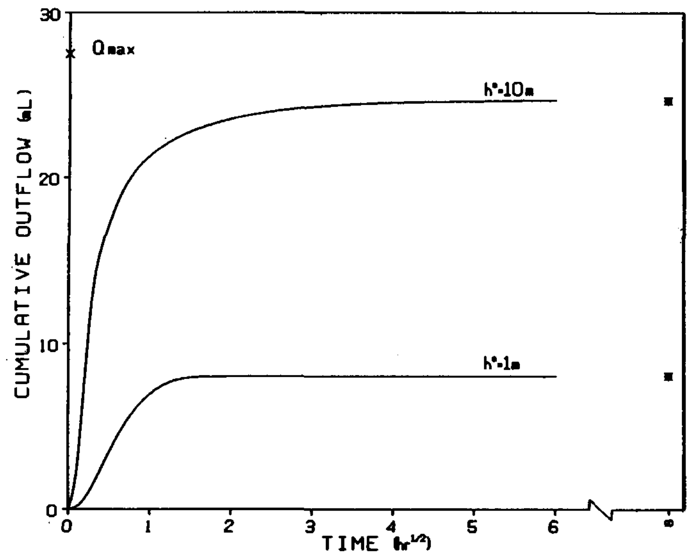

Fig. 1. Cumulative outflow with time from sandy loam for h^a = 1 and 10 m. *indicates outflow at equilibrium $Q(t_\infty)$.

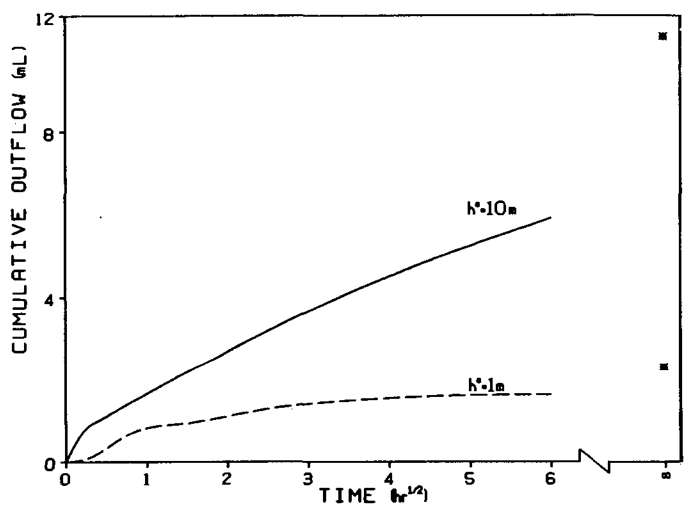

Fig. 2. Cumulative outflow with time from lay loam for h^a = 1 m and 10 m. *indicates outflow at equilibrium $Q(t_\infty)$. Q_{max} = 19.2 mL.

ipated that the probability of nonuniqueness will increase as $Q(t_N)$ diminishes relative to the equilibrium outflow volume $Q(t_\infty)$, where t_∞ is the time to effectively reach equilibrium. The probability of nonuniqueness is also expected to increase as $Q(t_N)$ diminishes relative to the total drainable volume of water in the column Q_{max} that corresponds to a decrease in water content from θ_s to θ_r. For a given pressure increment this suggests the desirability of collecting data over the entire outflow process $0<t<t_\infty$. On the other hand, minimizing t_N allows a reduction in experimental effort and computer time. As a compromise between these two requirements we employ transient data for the first hours of outflow supplemented by the total volume of outflow at equilibrium $Q(t_\infty)$. This means that experiments must be continued to equilibrium. However, the frequency of observation after the first hours of the experiment may be diminished. Also, since $h(x,t_\infty)$ is known from the imposed boundary conditions, the corresponding moisture content distribution can be obtained directly from Eq. [4], thus allowing $\hat{Q}(t_\infty)$ to be calculated with Eq. [3] without the need to solve the flow equation to large times.

Further details on the numerical procedures and documentation of the FORTRAN IV program ONESTEP which couples the nonlinear least-squares analysis with the numerical solution of the flow problem are given by Kool et al. (1985). Machine readable copies of the program are available from the authors on request.

Table 1. Assumed van Genuchten model parameters for hypothetical soils in numerical experiments.

Soils	θ_s	θ_r	K_s	α	n
	$m^3 m^{-3}$		$m s^{-1}$	m^{-1}	
Sandy loam	0.47	0.17	8.7×10^{-6}	1.00	2.00
Clay loam	0.45	0.24	6.9×10^{-9}	0.67	1.395

SOLUTION UNIQUENESS

The parameter identification procedure is examined for two hypothetical soils with contrasting hydraulic properties. Van Genuchten model parameters corresponding approximately to those of a sandy loam and a clay loam soil were chosen (Table 1). For brevity, we will refer to the two hypothetical soils by these names. Outflow data for the two soils (Fig. 1 and 2) were generated with the numerical solution assuming 54-mm diam by 40-mm long soil cores and 5.7-mm thick porous plates with $K_p = 1.39 \times 10^{-8}$ m s^{-1}. Initial conditions were hydrostatic with $h_o=0$ at the vertical center of the core and outflow levels were taken to give h_L = 20 mm. Simulations were performed for pneumatic heads h^a of 1.0 and 10.0 m, and for outflow volumes collected over different time periods. Parameter estimation runs were carried out using different initial (α, n, θ_r) values chosen to represent the range in parameter values that can be expected for most natural soils. The iterative optimization procedure was continued until the relative change in each parameter became <1%. Results are summarized in Table 2 which gives initial and final (α, n, θ_r) values and the degree of divergence between predicted and "observed" outflow. The latter is expressed as the proportion of variance of predicted outflow that is not attributable to its linear regression on observed outflow (Snedecor and Cochran, 1967) represented by the quantity $1 - r^2$ where r is the correlation coefficient. The number of times the flow equation was solved reflects the speed of convergence.

Sandy Loam

We first consider numerical inversion of the h^a = 1m outflow data for the sandy loam soil using $Q(t)$ values for $0<t\leq 3$ h and $t = t_\infty$. At t = 3 h $Q(t)/Q(t_\infty)$ > 0.99 (Fig. 1). Clearly, the results in Table 2 (Examples A1–A7) indicate that the input data in this case are insufficient to define a unique solution to the parameter estimation problem. Final parameter values exhibit marked heterogeneity and fits to the outflow data are rather unconvincing as evidenced by large $1 - r^2$ values, especially for cases A1, A2, A4, and A5, indicating that the solutions converge to local, rather than global minima. A comparison of predicted retention curves for the seven sets of final parameter values (Fig. 3) shows that over the observed range in pressure heads (0 to −1 m) the curves cluster into two groups with cases A1, A2, A4, and A5 along a spurious path and the curves for the other cases very close to the correct curve. Note that all curves yield essentially

Table 2. Solutions of parameter estimation problem.

Case	h_a	Outflow times	Initial estimates α	Initial estimates n	Initial estimates θ_r	Final estimates α	Final estimates n	Final estimates θ_r	$1 - r^2$	No. of trial solutions
	m	h	m^{-1}	–	$m^3 m^{-3}$	m^{-1}	–	$m^3 m^{-3}$	$\times 10^6$	
					Sandy loam					
A1	1	0–3, t_∞	5.00	1.10	0.150	3.11	1.159	0.001	2600	66
A2	1	0–3, t_∞	0.50	1.10	0.225	3.51	1.183	0.081	2900	41
A3	1	0–3, t_∞	1.00	3.00	0.075	0.83	1.945	0.080	70	21
A4	1	0–3, t_∞	5.00	1.50	0.150	4.66	1.260	0.214	5100	41
A5	1	0–3, t_∞	2.50	2.50	0.150	3.86	1.201	0.127	3100	41
A6	1	0–3, t_∞	0.50	3.00	0.005	0.77	1.936	0.035	300	30
A7	1	0–3, t_∞	5.00	2.75	0.225	1.18	2.439	0.260	340	48
B1	10	0–6, t_∞	5.00	1.10	0.150	1.00	2.002	0.170	0.08	29
B2	10	0–6, t_∞	0.50	1.10	0.225	1.03	1.940	0.166	7.8	25
B3	10	0–6, t_∞	1.00	3.00	0.075	0.99	1.985	0.169	1.0	21
B4	10	0–6, t_∞	5.00	1.50	0.150	1.00	1.997	0.170	0.15	27
B5	10	0–6, t_∞	2.50	2.50	0.150	1.00	2.011	0.171	0.74	43
B6	10	0–6, t_∞	0.50	3.00	0.005	1.02	2.001	0.170	0.20	17
B7	10	0–6, t_∞	5.00	2.75	0.225	1.35	3.647	0.194	1300	44
					Clay loam					
C1	1	0–6, t_∞	0.50	1.50	0.300	0.83	1.477	0.298	160	16
C2	1	0–6, t_∞	1.00	1.40	0.200	0.60	1.367	0.207	20	21
C3	1	0–6, t_∞	0.50	1.20	0.250	0.59	1.371	0.199	50	43
C4	1	0–6, t_∞	2.00	1.60	0.150	0.39	1.297	0.018	560	51
C5	1	0–6, t_∞	2.50	2.00	0.150	0.56	1.343	0.172	410	47
D1	10	0–6, t_∞	0.50	1.50	0.300	0.68	1.391	0.240	8.6	21
D2	10	0–6, t_∞	1.00	1.40	0.200	0.64	1.374	0.229	0.52	25
D3	10	0–6, t_∞	0.50	1.20	0.250	0.59	1.337	0.206	2.6	34
D4	10	0–6, t_∞	2.00	1.60	0.150	0.75	1.458	0.264	3.3	17
D5	10	0–6, t_∞	2.50	2.00	0.150	0.78	1.487	0.273	5.5	40
E1	10	0–12, t_∞	0.59	1.50	0.300	0.67	1.392	0.238	0.34	21
E2	10	0–12, t_∞	1.00	1.40	0.200	0.63	1.362	0.223	4.2	21
E3	10	0–12, t_∞	0.50	1.20	0.250	0.65	1.382	0.234	0.90	25
E4	10	0–12, t_∞	2.00	1.60	0.150	0.70	1.421	0.251	2.2	36
E5	10	0–12, t_∞	2.50	2.00	0.150	0.68	1.403	0.244	0.27	102

the same water content at $-h = h^a = 1$ m corresponding to $Q(t_\infty)$. At lower pressure heads, the curves diverge erratically leading to large errors in $\theta(h)$ predictions at potentials much beyond the range encountered experimentally.

This nonuniqueness for the sandy loam with $h^a = 1$ m may be attributed to the fact that experimental data span such a narrow range of soil water contents: $Q(t_\infty)/Q_{\max} = 0.29$. By contrast, for $h^a = 10$ m $Q(t_\infty)/Q_{\max} = 0.89$. Parameter estimation trials for $h^a = 10$ m outflow data with $0 < t \leq 6$ h and t_∞ were carried out using the same starting values as before. At $t = 6$ h the soil is quite close to equilibrium with $Q(t)/Q(t_\infty) = 0.97$. Unlike the $h^a = 1$m experiments, we now obtain excellent agreement between predicted and observed outflow and between predicted and actual parameter values (cases B, Table 2) in all cases except B7 which used initial values (5.0, 2.75, 0.225). The corresponding solution (1.35, 3.647, 0.194) differs considerably from the correct set and clearly does not represent an absolute minimum on the response surface since $1 - r^2$ is large compared to the other solutions. However, in absolute terms the deviations are still quite small and could go unnoticed if we were dealing with real soils, as opposed to the hypothetical soils considered here, where agreement between calculated and observed results will always be less than perfect.

The results for sandy loam above indicate that even for the larger pressure increment, the outflow data do not provide sufficient information to uniquely determine the three unknown parameters. On the positive side, however, it may be noted that only one case of nonuniqueness was observed. Furthermore, the solution (1.35, 3.647, 0.194) represents hydraulic properties which may be questioned on physical grounds since they are more likely for a sand than for a sandy loam

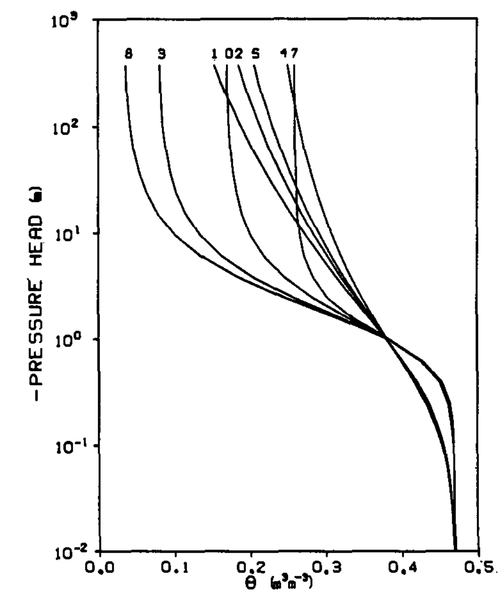

Fig. 3. Predicted retention curves for cases A1 to 7 of Table 2 for $h^a = 1$ m outflow experiments on sandy loam soil. Curve 0 represents correct $\theta(h)$ relationship.

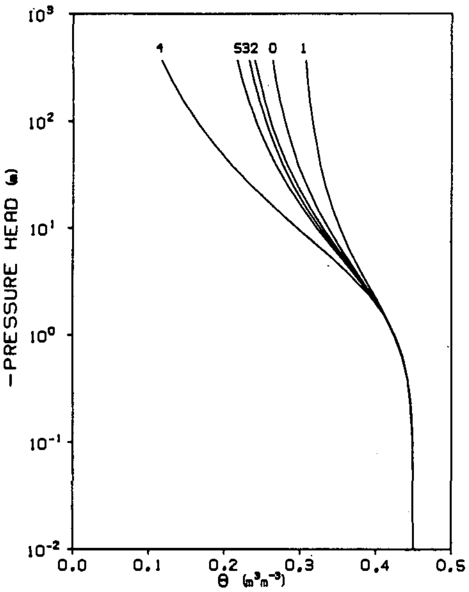

Fig. 4. Predicted retention curves for cases C1 to 5 of Table 2 for h^a = 1 m outflow experiments on clay loam soil. Curve 0 represents correct $\theta(h)$ relationship.

soil. Finally, we observe that good results were obtained in all cases where initial parameter estimates were reasonably close to the true values. This suggests that for the sandy loam, nonuniqueness would not be a serious problem in practice.

Clay Loam

The sandy loam example showed that initial parameter estimates can influence the results of the parameter estimation procedure. Fortunately, the range in possible parameter values for a given soil is rather narrow and reasonably close first estimates can be obtained from the texture of a sample. It is thus justified to use only initial parameter values that represent reasonable guesses in solving the inversion problem. Values were so chosen for the hypothetical clay loam soil.

We consider first the h^a = 1m outflow experiments employing $Q(t)$ for $0<t\leq 6$ h and t_∞. At t = 6 h $Q(t)/Q(t_\infty)$ = 0.70. For five cases with different initial values, final parameter estimates yield reasonably good fits to observed outflow data (cases C, Table 2). Whereas the final parameter estimates exhibited some heterogeneity, essentially identical $\theta(h)$ predictions were obtained (Fig. 4) over the experimental range in h from 0 to −1 m. For $h < -1$ m, predictions diverge markedly, reflecting nonuniqueness associated with the narrow range in water contents during the h^a = 1m outflow experiment for which $Q(t_\infty)/Q_{\max}$ = 0.12.

For the h^a = 10 m experiment on the clay loam $Q(t_\infty)/Q_{\max}$ increases to 0.53. Initially we employ as input to the inversion problem the outflow volumes $Q(t)$ for $0<t\leq 6$ h and t_∞, as well as the same combination of initial parameter values as used for the h^a = 1 m experiments. Solutions for all cases result in good agreement with measured outflow data, (cases D, Table 2). Also, variations in fitted parameters are less than were found for the h^a = 1m case. However, differences in fitted θ_r values still cause predicted $\theta(h)$ and $K(h)$ curves to diverge at pressure heads ≤ -10

Table 3. Sensitivity of parameter estimation problem solution to random error in input data for sandy loam.†

	I (p = 0.02)		II (p = 0.05)		III (p = 0.15)	
	Rep a	Rep b	Rep a	Rep b	Rep a	Rep b‡
Final α	0.96	1.01	0.88	0.90	0.78	1.84
Final n	1.957	2.115	1.748	1.745	1.934	4.913
Final θ_r	0.168	0.178	0.146	0.145	0.172	0.190
$1 - r^2 (\times 10^6)$	850	860	7000	2000	8800	-
No. trials	17	21	25	27	44	29

† Outflow data $Q_p(t)$ for t = 0 to 6 h and t_∞, h^a = 10 m. Units of α in m⁻¹, θ_r in m³ m⁻³, n dimensionless.
‡ Last selected parameter values. Execution stopped because of persistent oscillations in the solution of direct problem.

m. Note that $Q(t/Q(t_\infty)$ for this soil was only 0.35 when using input data with outflow to t = 6 h. The input data thus cover a much smaller part of the outflow process than was the case with the sandy loam soil. Therefore, the inversion problem was solved again for the same initial parameter values using outflow data up to 12 h, and also including $Q(t_\infty)$. After 12 h $Q(t)/Q(t_\infty)$ = 0.44. This leads to solutions (cases E, Table 2) that are very close to the correct parameter values and all closely approximate the "true" hydraulic properties of the soil. Except for case E5, speed of convergence is generally quite good.

SENSITIVITY TO EXPERIMENTAL ERROR

We turn now to an investigation of the effects of random error (noise) in the input data on the parameter estimation problem solution. We utilize the hypothetical outflow data for the sandy loam soil, upon which we overlay random errors using:

$$Q_p(t_i) = Q_o(t_i)[1 + 2p\,(R - 0.5)] \qquad [9]$$

where $Q_p(t_i)$ denotes the outflow with added random error at times t_i = 0 to 6 h and also includes $Q(t_\infty)$, $Q_o(t_i)$ represents the exact outflow, R is a random number between 0 and 1, and p is the relative error. To simulate measurement error of 2, 5, and 15%, we successively set p to 0.02 (case I), 0.05 (case II) and 0.15 (case III), respectively. For the solution of the inversion problem we use initial parameter values (2.50, 1.50, 0.150). These values represent "best guess" estimates. When these initial values were used with the exact outflow data, the solution quickly converged to exactly the correct parameter values, requiring the flow equation to be solved 17 times. At each noise level we generated two series of outflow data denoted as a and b, each consisting of 10 data points. Two series were used to get some indication about the variation that might occur at a given level of error. Table 3 shows that the inversion problem is sensitive to errors in input data. The effect on the parameter estimates is small but noticeable at the 2% level, greater at the 5% level, and quite dramatic at the 15% error level. For case IIIa, errors in the parameters are relatively small but deviations between predicted outflow and input data remain quite high as can be seen from the value of $1 - r^2$. For case IIIb, the solution failed to converge at all and program execution was interrupted because the selected parameter values led to persistent oscillations in the solution of the flow equation. For the chosen time and space discretiza-

Table 4. Solutions of parameters estimation problem for sandy loam with various degrees of error in input K_s values.†

$\hat{K}_s/K_s$	Final parameter values†		$1 - r^2$ ($\times 10^6$)	No. of trial solutions
1.25	α	1.18	90	33
	n	1.956		
	θ_r	0.171		
0.75	α	0.83	90	40
	n	2.046		
	θ_r	0.169		
1.50	α	1.31	80	31
	n	1.919		
	θ_r	0.172		
0.50	α	0.62	580	30
	n	2.144		
	θ_r	0.164		
2.0	α	1.53	130	27
	n	1.675		
	θ_r	0.150		

† Outflow data $Q(t)$ for $t = 0$ to 6 h and t_∞. Units of α in m^{-1}, θ_r in m^3 m^{-3}, n dimensionless.

tion, numerical difficulties were encountered for large values of n when $\theta(h)$ and $K(h)$ tend towards step functions.

In addition to experimental errors in outflow volumes, significant errors are also possible in the input values for K_s; such errors may be due to analytical inaccuracies or to the sensitivity of K_s to small changes in soil structure during testing. To evaluate the effects of uncertainty in K_s we carried out parameter estimation analyses for $h^a = 10$ m outflow data for the sandy loam soil assuming error-free outflow measurement using initial parameter values of (0.025, 1.5, 0.15) and employing erroneous input K_s values. Results are given in Table 4 for $\hat{K}_s/K_s$ varying between 0.5 and 2.0, where $\hat{K}_s$ is the input value and K_s is the true value. For errors of ± 25% in K_s, effects on final parameter estimates are relatively minor. However, using input K_s values that are either half or twice as large as the correct value results in serious errors in parameter estimates.

CONCLUSIONS

The determination of soil hydraulic properties by parameter estimation allows for considerable freedom in choosing experimental boundary conditions and measurements to be used as input data. It has been our approach to choose boundary conditions and measurements in such a way that the experimental procedure can be kept simple, yet applicable to a variety of soils, rather than search for a method that is optimum in terms of uniqueness and sensitivity to data variability. Results of Zachman et al. (1981) suggest that cumulative drainage data may be an attractive choice from either point of view. Although our investigation of solution uniqueness is by no means exhaustive, results for two hypothetical soils suggest that nonuniqueness, while of some concern, need not be a serious problem. Good results can be obtained for one-step pressure outflow experiments using cumulative outflow with time as input data if the pressure increment is selected to yield a relatively low final reduced water content and if input data include a reasonably large portion of the transient flow process. Using cumulative outflow $Q(t)$ to at least about 50% of $Q(t_\infty)$ and including as well the value $Q(t_\infty)$ appear to be generally sufficient for accurate results.

Initial parameter values should be reasonably close to their actual values to reduce chances of finding an erroneous solution and to enhance the speed of convergence. An approximate range for α and n has already been given. Using "average" initial values, for instance $\alpha = 2.50$ m^{-1}, $n = 1.75$ and $\theta_r = 0.150$, should give good results for most medium textured soils. These initial values can be suitably adjusted for soils with different particle size distributions. As a check on the results, it should be verified that a solution of the identification problem corresponds to reasonable $\theta(h)$ and $K(h)$ for the particular soil. In case of uncertainty, we recommend that the inversion process be repeated with different initial estimates.

Our results show that solutions of the parameter estimation problems are sensitive to errors in measured data. This is in contrast to findings by Zachman et al. (1982), who studied a gravity drainage experiment and found that relative errors in input data were apparently dampened in the solution process. Our simulations suggest that parameter estimates are more sensitive to errors in outflow measurements than to errors in input saturated conductivity values. On the other hand, uncertainty in unsaturated conductivity due to experimental error and/or variations in actual saturated conductivity during testing may, in practical circumstances, be considerably larger than errors in observed outflow. Also, we evaluated both sources of error independently, while in practice they will be compounded. All this emphasizes the need for accurate experimental measurements. Convergence speed of the optimization routine is variable and sensitive to small changes in input data and/or initial parameter values (reflecting the irregularity of the response surface). The average number of times the flow equation had to be solved for all cases discussed in this study was 34. This corresponds to an average CPU-time of just below 1 min on the IBM 3081 computer used. In one case (case E5, Table 2) the solution was found to converge very slowly. In practice, excessively long computer runs are avoided by setting an upper limit to the number of function evaluations allowed. If the solution fails to converge in the allowed number of evaluations, we suggest that the solution process be started anew with different initial parameter values.

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