Effective Unsaturated Hydraulic Conductivity for Computing One-Dimensional Flow in Heterogeneous Porous Media

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ABSTRACT

Steady-state and transient one-dimensional unsaturated flow in vertically stratified porous media are examined. Saturated hydraulic conductivity and the alpha parameter of the exponential hydraulic conductivity function were assumed to vary from soil layer to soil layer. The use of effective unsaturated hydraulic conductivity to compute matric potential in the soil profile is demonstrated. Results indicate that soils with vertical variation in these hydraulic parameters can be represented by a single effective parameter set. The harmonic mean of the set of hydraulic parameters for each of the soil layers produces accurate results when used as an effective parameter for unsaturated transient flow with layering perpendicular to the direction of flow. A direct relation for calculating specific moisture capacity based on hydraulic and moisture characteristics of the soil is also presented.

INTRODUCTION

Uncertainty in input parameters for hydrologic models creates difficulty in interpreting the output of these models. Systems with large one-, two-, and three-dimensional heterogeneity are often impossible to represent deterministically. The problem of assessing this uncertainty can, however, be partially solved by representing these systems stochastically. Previous investigations have applied the stochastic approach to steady-state saturated and unsaturated groundwater flow. One approach has been to assume a random spatial variability in hydraulic conductivity. For unsaturated flow, a functional form relating the hydraulic conductivity to the matric potential of the soil is assumed. Gardner (1958) presented an exponential form:

$$K = Ksat \exp(\alpha \psi) \quad [1]$$

where K is the unsaturated hydraulic conductivity (L/T), Ksat is the saturated hydraulic conductivity (L/T), α is a constant related to pore-size distribution (1/L), and ψ is the soil-water matric potential (L).

In a stochastic representation of the soil system, Ksat and α are random variables. This technique is particularly well suited for analyzing heterogeneous soil profiles. In these cases, representing the soil deterministically is difficult. Parameters associated with the soil layers can be represented stochastically with a specified autocorrelation between the parameters. Simulations can be then performed to analyze the effects of the heterogeneity.

Bouwer (1969) demonstrated the application of effective parameters for steady-state saturated flow. Andersson and Shapiro (1983), Yeh et al. (1985a,b,c), and Yeh (1989) applied stochastic techniques to steady-state unsaturated flow. Bresler and Dagan (1983) analyzed infiltration into an unsaturated soil with horizontal variability in Ksat. The analysis assumed Ksat was a lognormally distributed random variable and the other hydraulic characteristics of the soil were spatially constant. Given these constraints, they found effective properties to be meaningful only under very restricted and special conditions such as steady gravitational flow. They concluded the traditional deterministic approach for solving the flow equations cannot be justified for solving flow problems in fields with horizontal spatial variability.

Our research continues upon the work of Bresler and Dagan by examining heterogeneity in the hydraulic conductivity in the vertical direction. This work examines variability in the exponent alpha of equation [1] as well as variability in saturated hydraulic conductivity. This research evaluates if deterministic approaches are being correctly applied to unsaturated flow for fields with vertical, as well as horizontal, spatial variability. The current analysis demonstrates and evaluates the application of effective soil parameters for transient unsaturated flow in heterogeneous porous media.

Objectives

The objectives of this study were 1) to evaluate the applicability of effective parameters in one-dimensional (1-D) analysis of vertical transient unsaturated flow in a vertically stratified soil profile; and 2) to evaluate methods for determining effective parameters for the equivalent vertical profile.

METHODS

Background and Equations

This study investigated unsaturated 1-D flow in a layered soil profile using Richards' equation:

$$C \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left[K \frac{\partial}{\partial z}(\psi - z)\right] \quad [2]$$

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where

C = specific moisture capacity (1/L),
ψ = matric potential (L),
t = is time,
K = unsaturated hydraulic conductivity (L/T),
z = the vertical coordinate, positive downward (L).

Specific moisture capacity is defined as

$$C = \frac{d\theta}{d\psi} \quad [3]$$

where θ is the volumetric moisture content of the soil (L^3/L^3). Equation [1] was used to determine the hydraulic conductivity. Specific moisture capacity was calculated from equations presented by Russo (1988):

$$S = \frac{\theta - \theta r}{\theta sat - \theta r} = (\exp(.5\alpha\psi)\,(1-.5\alpha\psi))^{\beta} \quad [4]$$

or

$$\theta = S\,(\theta sat - \theta r) + \theta r \quad [5]$$

where

β = 2/(m+2)
S = is effective saturation,
m = a parameter which accounts for the dependence of the tortuosity and the correlation factors on the water content,
θsat = is saturated moisture content,
θr = is residual moisture content.

α and Ψ are as previously defined. Specific moisture capacity can then be calculated as

$$C = (\theta sat-\theta r)\,[\beta(\exp(.5\alpha\psi))^{\beta-1} *(-.25\alpha^2\psi \exp(.5\alpha\psi))] \quad [6]$$

The finite-element solution developed by Khaleel and Yeh (1985) was used to solve equation [2]. The program uses linear basis functions and a Galerkin finite-element weighting scheme. Since the hydraulic conductivity and the specific moisture capacity are both functions of Ψ, one must iterate to solve equation [2]. The Newton-Raphson iteration technique was incorporated in the finite element program to ensure convergence. This iteration technique requires the derivative of C with respect to Ψ. The derivative is calculated from equation [6] as

$$\frac{dC}{d\psi} = (\theta sat-\theta r)[\beta(\beta-1)(\exp(.5\alpha\psi)] \quad [7]$$

$$*(1-.5\alpha\psi))^{\beta-2}(-.25\alpha^2\psi \exp(.5\alpha\psi))^2 + (\beta(\exp(.5\alpha\psi)(1-.5\alpha\psi))^{\beta-1}$$

$$*(-.25\alpha^2\exp(.5\alpha\psi)-.125\alpha^3\psi \exp(.5\alpha\psi))]$$

The functional forms provided by equation [6] and [7] increase the computational efficiency of the computer program considerably.

TABLE 1. Number of layers and mean and variance of the saturated hydraulic conductivities and alpha parameters for the two simulated cases

	Number of Layers	Ksat mean (cm/hr)	Ksat variance (cm^2/hr^2)	α mean (1/cm)	α variance ($1/cm^2$)
Case 1	20	4.9	7.3	0.038	5.6×10^{5}
Case 2	1000	5.2	2.7	0.040	9.6×10^{6}

Simulations

To simulate a heterogeneous soil profile, several vertical layers were assumed. Following a procedure described by Yeh (1989), the natural log of Ksat (ln Ksat) and an α value were randomly generated for each layer. The values were assumed correlated between one layer and the next. Ln Ksat and α were assumed to be perfectly correlated. An exponential autocorrelation function was used.

Two different cases were examined in the simulation. The cases were designed to represent soil systems with different degrees of hydraulic heterogeneity. The simulations were analyzed to determine how the different degrees of heterogeneity affected the results. Case 1 represented a soil with large variability between the layers. Case 2 had significantly less variability between the soil layers. One can view the second soil as a relatively homogeneous soil with small variability depending on the scale chosen or the scale at which measurements are taken. For each case, the soil was divided into layers and a Ksat and an α were assigned to each layer. The number of soil layers and the mean and variance of the assigned values for the two cases are presented in Table 1.

To avoid adding additional complexity to the analysis, θsat, θr, and m were assumed to be constant for the entire profile and for both of the cases. For heterogeneous soils these parameters would be variable. This assumption, however, allowed the separation of the effects of the variation in Ksat and α from the effects of variation in θsat, θr, and m. Russo and Bressler (1982) indicated that the impact of the variability of the other hydraulic parameters is limited in comparison to the impact of variation in Ksat. θsat, θr, and m chosen for both cases were 0.40, 0.10, and 0.50, respectively.

A column length of 2 000 cm was chosen for both cases. The initial pressure at each of the nodes was obtained from a steady-state solution with a flux equal to 0.1 cm/h and a lower boundary condition of constant matric potential equal to 0 cm. A constant flux equal to 1 cm/h was used as the top boundary condition for the transient and final steady-state runs. The lower boundary condition remained the same for the transient and final steady-state runs.

RESULTS

Effective Parameter Methods

Simulation results for the two cases are presented in Figs. 1 and 2. The initial and final steady-state Ψ profiles are presented along with three of the intermediate transient profiles. The larger variability in the input parameters of case 1 translated into larger variability in the Ψ profile.

Five different methods were used to estimate effective

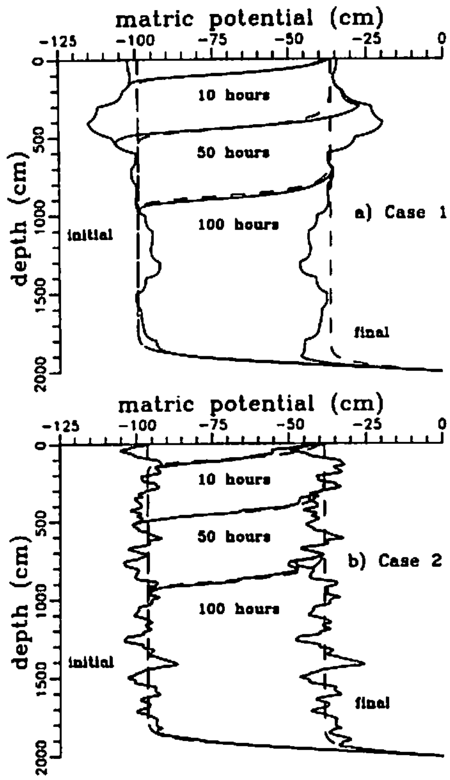

Fig. 1—Heterogeneous pressure profiles (solid) and effective pressure profiles calculated by the harmonic mean of Ksat and alpha (dashed) for Case 1 and Case 2.

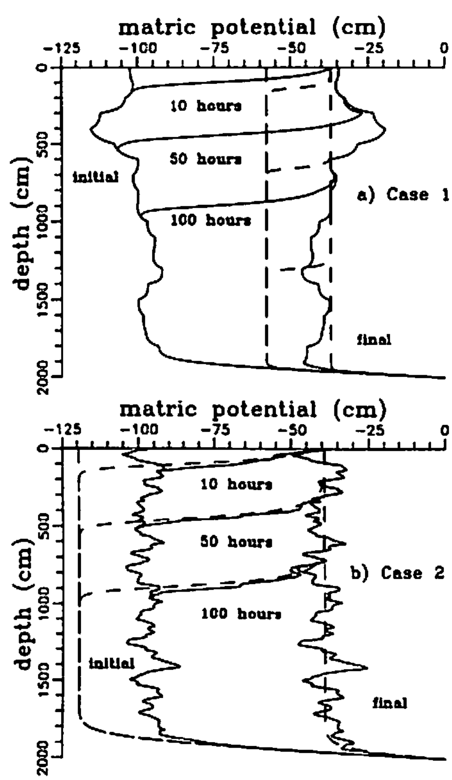

Fig. 2—Heterogeneous pressure profiles (solid) and effective pressure profiles calculated by the Ksat and alpha parameters obtained through inverse fitting based on the final steady-state pressure profile (dashed) for Case 1 and Case 2.

parameters for the heterogeneous profiles. Of the five methods chosen, three involved calculating the mean of the heterogeneous Ksat and α parameter set. The mean methods chosen were the arithmetic mean (AM), the harmonic mean (HM), and the geometric mean (GM). Two estimates were determined through inverse fitting methods as described by Yeh (1989). The inverse fitting methods used the criteria

$$\sum_{i=1}^{n} (H_i - \psi_i)^2 = \text{minimum}$$

where H_i is the potential at the i^{th} depth calculated from the effective parameters, Ψ_i is the potential calculated from the simulation using the heterogeneous profile parameter set, and n is the total number of depths. In the inverse procedure, Ksat and α values were adjusted to arrive at the minimum. The inverse procedure was used to fit the initial steady-state (IFI) and the final steady-state Ψ profiles (IFF), and an effective Ksat and α were determined for each. The effective parameters determined for Cases 1 and 2 are shown in Table 2. The inverse fitting method produced estimates for Ksat and α considerably different from thse produced by the mean methods.

The ψ profiles calculated by the harmonic mean method for Case 1 are shown in Fig. 1a. Similar results were obtained using the other mean methods. The harmonic mean method produced reasonable representations of the heterogeneous Ψ profiles (Fig. 1a). The profiles calculated with inverse estimates did not fit as well as those calculated with mean methods. The potential profiles calculated by inverse estimates based on the final steady-state heterogeneous profile are shown in Fig. 2a. This ψ profile fit very poorly for all times except the final condition.

The ψ profiles calculated by the harmonic mean method for Case 2 are shown in Fig. 1b. Again, as in Case 1, the equivalent Ψ profiles calculated with the three mean-parameter estimates produced good representations of the heterogeneous Ψ profile. The Ψ profile calculated when the effective parameters were estimated by the inverse fitting method again fit poorly. The technique which fit the initial steady-state profile failed to predict the other profiles accurately. As shown in Fig. 2b, the technique which fit the final steady-state profile also failed to predict the other profiles accurately.

The variance of the errors between the heterogeneous and the effective Ψ profile point values was calculated for each method. The variance was calculated as

TABLE 2. Effective parameters used for the equivalent homogeneous profile of Cases 1 and 2

method	abbreviation	Case 1 Ksat (cm/hr)	Case 1 α (1/cm)	Case 2 Ksat (cm/hr)	Case 2 α (1/cm)
arithmetic mean	AM	4.9	0.0381	5.2	0.0400
harmonic mean	HM	3.8	0.0366	4.7	0.0399
geometric mean	GM	4.3	0.0374	4.9	0.0400
inverse fitting based on initial conditions	IFI	2.6	0.0320	2.5	0.0330
inverse fitting based on final conditions	IFF	59.5	0.1100	3.1	0.0287

TABLE 3. Variance of the errors (cm^2) between the heterogeneous and effective potential point values for each of the estimation methods at each of the calculated times for Case 1

Method	Time (hours) 0	10	50	100	∞
AM	33.0	34.3	41.5	86.2	68.2
HM	30.7	30.3	15.1	36.5	46.4
GM	29.6	30.0	25.2	58.0	50.1
IFI	31.4	32.4	23.6	30.7	95.3
IFF	1718.0	1643.0	1382.0	1145.0	42.9

TABLE 4. Variance of the errors (cm^2) between the heterogeneous and effective potential point values for each of the estimation methods at each of the calculated times for Case 2

Method	Time (hours) 0	10	50	100	∞
AM	13.3	14.8	15.1	16.6	21.4
HM	11.8	13.2	13.3	15.5	18.6
GM	11.3	12.8	14.8	18.6	18.6
IFI	10.8	19.9	43.4	86.4	152.6
IFF	469.8	448.1	353.9	266.4	18.0

$$S_e^2 = \frac{\Sigma (H_i - \psi_i)^2}{n-2} \qquad [8]$$

where S_e^2 is the variance of the errors, and H_i, ψ_i, n are as previously defined. The variances calculated for the different estimation methods are shown in Tables 3 and 4. A comparison of the variance of errors for Case 2 (Table 4) to those for Case 1 (Table 3) indicates that the overall variance in Case 2 was less than the overall variance of Case 1.

Mass balance was also calculated to evaluate the accuracy of the equivalent methods. The outflow rates from each of the methods at each of the observed times were equivalent to those of the hetergeneous profile. The total water volume in the soil profile for each of the methods at 0 h, 100 h, and ∞ h is shown in Tables 5 and 6. Similar results were observed at 10 and 50 hours. The mass balance of the inverse fitting methods was not as accurate as that of the mean methods (Tables 5 and 6). This inaccuracy can be attributed to the poor estimate of alpha which altered the matric pressure-moisture content relation for the soils.

Equilibrium Flux Approach

Field data (Greenholtz et al., 1988; Russo and Bresler, 1980; Byers and Stephens, 1983) has shown ln Ksat and α to be spatially correlated in vertical field profiles. Yeh (1989) points out that for cases where ln Ksat and α are perfectly correlated for a layered soil system, there will exist a steady-state equilibrium flux at which the profile will behave as though it is homogeneous. That is, the matric potential curve will correspond to a unit gradient condition where the matric potential above the capillary fringe is constant. This constant matric potential, when used with any pair of Ksat and α values for the hetergeneous profile, will yield an unsaturated hydraulic conductivity equal to the equilibrium flux. This is attributed to the perfect correlation between ln Ksat and α. This flux will occur when the mean matric potential in

TABLE 5. Volume of water (cm) in the soil for the heterogeneous profile (HET) and for each of the equivalent methods at the initial, 100 hour, and final times for Case 1

Method	Initial volume (cm)	Initial error (%)	100 hours volume (cm)	100 hours error (%)	Final volume (cm)	Final error (%)
HET	522.5	0	612.5	0	718.7	0
AM	509.8	-2.4	599.7	-7.5	708.8	-9.9
HM	530.5	1.5	620.4	1.3	731.3	1.8
GM	520.1	-0.5	609.9	-0.4	720.2	0.2
IFI	561.9	7.5	651.9	6.4	760.1	5.8
IFF	353.6	-32.3	443.0	-27.7	488.9	-32.0

TABLE 6. Volume of water (cm) in the soil profile for the heterogeneous profile (HET) and for each of the equivalent methods at the initial, 100 hour, and final times for Case 2

Method	Initial volume (cm)	Initial error (%)	100 hours volume (cm)	100 hours error (%)	Final volume (cm)	Final error (%)
HET	511.2	0	601.0	0	710.9	0
AM	506.4	-0.9	596-2	-0.8	705.2	-5.7
HM	513.6	-0.9	596.2	-0.8	705.2	-5.7
GM	510.0	-0.2	599.9	-0.2	709.5	-0.2
IFI	566.4	10.8	656.5	0.9	764.0	37.3
IFF	549.6	7.5	639.5	6.4	748.2	37.3

the profile equals the coefficient of correlation between ln Ksat and α. The coefficient was 70.5 cm for Case 1, and 305.4 cm for Case 2. This corresponded to an equilibrium flux of 0.294 cm/h and 2.4 x 10^{-5} cm/h for Cases 1 and 2, respectively. Above and below this flux the variation in the steady-state matric potential curve will diverge from this minimum.

If the effective parameter sets calculated in this analysis are used to calculate the equilibrium flux for these matric potentials, one might expect the best estimates to produce a flux equal to these equilibrium fluxes for the hetergeneous profiles. For the two cases, the harmonic mean parameter set produced a flux of 0.298 cm/h and 2.36 x 10^{-5} cm/h, and the geometric mean produced a flux of 0.310 cm/h and 2.46 x 10^{-5} cm/h for Cases 1 and 2, respectively.

Unit Gradient Approach

Another method which can be used to determine the effective hydraulic parameters is to assume a unit gradient in the soil profile. In this case,

$$\frac{\partial y}{\partial z} = 0; \frac{\partial z}{\partial z} = 1.$$

In the unit gradient approach, the flux is equal to the hydraulic conductivity. As described by Yeh (1989), if one plots the flux vs. the mean matric potential above the capillary fringe for the heterogeneous profile, the effective hydraulic parameters can be calculated from the lines passing through the data points. The steady-state fluxes simulated in this analysis yielded the results in Table 7. The values obtained through the unit gradient approach are in close agreement with those calculated from the mean methods.

TABLE 7. Effective hydraulic parameters calcaulated by the unit gradient approach for Cases 1 and 2

	Ksat	a
Case 1	3.7	0.0354
Case 2	5.0	0.0397

DISCUSSION

The results indicate a wide variability in the accuracy of the equivalent methods. This variability can be seen by examining Tables 3 and 4. The three equivalent methods which used the mean estimation techniques were generally quite accurate in representing the ψ profile. As expected, the methods had better accuracy for Case 2 where the soil variation was less. The two methods which used inverse fitting were not as accurate, with larger errors when applied to different conditions than those at which they were fit. Perhaps a better inverse fitting method would have been to fix either Ksat or α while adjusting the other parameter.

Of the equivalent methods, the harmonic and geometric mean methods produced the most accurate results. Theory based on Darcy's law for steady-state saturated flow has shown that the effective hydraulic conductivity for vertically-layered flow such as this would be the harmonic mean of the saturated hydraulic conductivities of the layers. Results of this study are consistent with this theory, indicating that the harmonic mean is also applicable for some cases of unsaturated transient flow. These results also indicate that the accuracy of the effective parameters are not greatly influenced by matric potential. That is, the effective parameters which produced the best estimates of the matric potential curve at the initial condition produced good estimates at other times as well. This does not include the effective parameters obtained through the inverse fitting methods.

The results have significant implications with regard to using field data to analyze transient flow into unsaturated soils. First and most importantly, since effective hydraulic pararmeter sets appear to adequately simulate the heterogeneous conditions, it may not be necessary to precisely evalute the heterogeneous profile characteristics. In cases of large variability in the profile, evaluating the parameter set for each soil layer may be an insurmountable task. However, these results indicate that if the statistical parameters of the profile as a whole can be evaluated, one can use effective parameter sets to characterize flow into this system. In addition, since the accuracy of effective parameter sets appears to be fairly constant with respect to matric potential, field measurements of matric potential in the soil profile taken at one or two infiltration rates can be used to determine the effective parameter sets. These parameter sets can then be used to simulate other infiltration rates as well. A proposed field measurement technique is to apply the unit gradient approach using the mean matric potential and steady-state flux determined in the field measurements. Since inverse fitting methods do not appear to work well, it will not be possible to use inverse fitting to determine effective parameters from a matric potential curve measured at a single steady-state flux rate. However, an inverse procedure proposed by Yeh (1989) using matric potential profiles measured at different steady-state flux rates may be more appropriate.

SUMMARY

Results presented here indicate that vertical spatial variability can be represented by equivalent homogeneous profiles for purposes of modeling unsaturated flow. How well the equivalent profile represents the heterogeneous profile depends upon the objectives of the simulation. Considerable variation exists between the ψ predictions calculated using the heterogeneous parameters and those calculated using equivalent homogeneous parameters (Fig.s 1 and 2). The equivalent homogeneous methods will not precisely predict the matric potential throughout the profile at all times. However, if the objective is to obtain a reasonable estimation of the flux throughout the soil and to predict an approximation of the ψ profile in the soil, equivalent homogeneous methods appear adequate.

The analyses performed during this study were limited and should not be assumed to apply to all cases of soil heterogeneity. Cases with larger variability and different column lengths may produce results significantly different from those presented here. Also, it is not known how hysterisis affects the process. Potential curves obtained on the drying phase of the soil may not fit as well as those discussed here. Further research is also required to determine how hydraulic conductivity values determined in steady-state laboratory experiments compare to the effective parameters determined in this study.

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