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Numerical modeling of observed effective flow behavior in unsaturated heterogeneous sands

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Abstract. The concept of effective parameters has been introduced in recent years to represent the spatial variability of natural soils in numerical simulation models. In the present study, effective hydraulic properties of unsaturated flow were investigated for the case of a two-dimensional heterogeneous laboratory tank. Hydraulic parameter estimates obtained from simple statistical averages, inverse procedures, and a stochastic theory were compared to effective retention and hydraulic conductivity characteristics measured for the whole tank at steady state. The applicability of the effective parameter estimates was investigated by comparing transient flow events monitored in the laboratory tank with simulated results based on those estimates. Capillary suction measurements were simulated reasonably well using several straightforward arithmetic and geometric statistical averaging approaches, whereas most averaging approaches simulated too slow a response in the outflow rate. An alternative approach involving a combination of arithmetic and geometric averaging of the measured values more closely simulated the observed relatively fast changes in outflow rate. Generally, the simulations based on the measurements of effective properties performed quite well, indicating that the fundamental concept of effective parameters may be valid for this type of heterogeneous soil system.

1. Introduction

Any attempt at modeling flow and transport in natural soils will be confronted with the issue of spatial variability of hydraulic properties due to soil heterogeneity. The presence of spatial variability in hydraulic properties of natural soils is well-documented; hydraulic properties have been shown to be variable in both vertical and horizontal planes, although more structure is often seen in the horizontal direction than in the vertical [*Russo and Bresler*, 1981; *Byers and Stephens*, 1983; *Greenholtz et al.*, 1988; *Jensen and Refsgaard*, 1991a, b, c; *McCord et al.*, 1991a, b; *Jensen and Mantoglou*, 1992]. When evaluating flow and transport phenomena in field soils, the fundamental question arises of how best to incorporate the effects of heterogeneity in numerical simulation models. A common approach is to use deterministic numerical models and attempt to incorporate the overall heterogeneity of the system such as layering while neglecting the small-scale heterogeneity. The considerable spatial variability of natural soils makes complete characterization of the hydraulic properties at the field scale an almost impossible task, as enormous amounts of data are required for proper representation of the actual heterogeneity. Even if the hydraulic properties somehow could be characterized, deterministic simulations would demand vast computational resources by requiring an extremely dense numerical grid system.

Alternatively, one could interpret the soil as an equivalent homogeneous medium with average (effective) hydraulic properties that are related to the local values of the heterogeneous system properties and thereby predict the average flow and transport behavior of the system. Studies by *Bresler and Dagan* [1981, 1983a, b] and *Dagan and Bresler* [1983] suggested that flow and transport in a heterogeneous soil cannot be predicted by the classical differential equations using "effective soil properties." However, these studies were limited to a decoupled one-dimensional stream-tube type approach, which is not a realistic analogue of a field situation. Flow and transport in natural soils is generally three-dimensional, often dominated by geological formations with some stratification that tends to promote lateral components.

When choosing to represent a heterogeneous soil by its homogeneous equivalent, the subsequent question of estimating the effective hydraulic properties representing this equivalent homogeneous medium arises. A straightforward approach would be to use simple statistical averages (arithmetic or geometric) of the local soil hydraulic properties, but such simple estimates may not be able to properly describe the complicated nonlinear flow and transport behavior in a heterogeneous soil system. Another option is to conduct transient laboratory or field experiments and then to apply some inverse method to obtain the effective properties. Existing inverse procedures are often accompanied by problems of nonuniqueness and correlation between individual parameters [e.g., *Kool et al.*, 1985; *Parker et al.*, 1985; *Toorman et al.*, 1992; *van Dam et al.*, 1992; *Wildenschild et al.*, 1997]; hence relatively well-defined boundary conditions and small measurement errors are important in order to apply this approach to transient experiments.

In recent years, stochastic models have become increasingly popular for describing flow and transport in heterogeneous soils. The stochastic models of *Yeh et al.* [1985a, b, c], *Mantoglou and Gelhar* [1987a, b, c] and *Mantoglou* [1992] have been tested on data from both field [*Jensen and Mantoglou*, 1992; *Polmann et al.*, 1988, 1991; *McCord et al.*, 1991a, b] and laboratory studies [*Yeh and Harvey*, 1990]. A laboratory analysis

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Table 1. *van Genuchten* [1980] Parameters for Both Retention and Unsaturated Hydraulic Conductivity Characteristics

			Retention-based		Conductivity-based			
	θ_s	θ_r	α	n	α	n	K_s	Case numbers
Sand type								
00	0.360	0.094	0.026	8.0	0.029	5.2	5.64×10^{-5}	
0	0.369	0.060	0.024	8.3	0.034	5.6	1.23×10^{-4}	
1	0.370	0.014	0.044	12.0	0.066	8.4	6.70×10^{-4}	
2	0.367	0.014	0.060	9.7	0.085	6.3	1.13×10^{-3}	
3	0.363	0.005	0.098	7.8	0.110	8.8	1.07×10^{-3}	
Measured effective (arith)	0.200	0.001	0.055	2.8	0.065	3.7	2.50×10^{-4}	1
Inverse estimate	0.366	0.022	0.061	3.3	0.061	3.3	2.50×10^{-4}	2
Stochastic (stratified) approach	0.366	0.022	0.066	4.8	0.069	19.0	1.40×10^{-4}	3
Arithmetic average	0.366	0.022	0.053	3.0	0.050	4.0	6.10×10^{-4}	4
Geometric average	0.366	0.022	0.066	4.8	0.080	5.3	3.55×10^{-4}	5
Arith./geom. (local)	0.366	0.022	0.053	3.0	0.080	5.3	3.55×10^{-4}	6
Arith./geom. (eff.)	0.200	0.001	0.055	2.8	0.068	3.8	2.50×10^{-4}	7
Arith./geom. (eff.) alt. θ_s	0.366	0.001	0.055	2.8	0.068	3.8	2.50×10^{-4}	8

Arith., arithmetic; geom., geometric; eff., effective; alt., alternate.

carried out by *Yeh and Harvey* [1990] for the case of one-dimensional flow in a layered soil column showed that the stochastic model was capable of providing reliable estimates of the effective unsaturated hydraulic conductivity. Unfortunately, one-dimensional analyses do not permit water to follow pathways of least resistance. Hence there is still a need to take laboratory assessments beyond one dimension, since flow in natural soils generally is multi-dimensional. Field experiments, however, are costly and difficult to carry out, and there are numerous uncertainties involved when carrying out this type of experiment in a natural soil. Thus, in order to carry out a more extensive test of the concept of effective parameters and associated stochastic theories under controlled conditions, *Wildenschild and Jensen* [this issue] investigated two-dimensional flow and transport in a well-defined heterogeneous soil system built into a laboratory flow flume. They derived effective unsaturated hydraulic properties directly under steady state conditions and compared these values to the properties of the individual homogeneous sands. The study showed that effective properties could be determined for such heterogeneous yet controlled soil systems. Not yet addressed was the important question of whether these measured effective properties could adequately represent the flow system; that is, how they would perform as input parameters to numerical models when modeling, for instance, transient flow.

Thus the objectives of the present study are to (1) test different parameter estimates, including simple statistical averages of the properties of the individual sands, inverse estimates derived from transient experiments, and estimates based on a stochastic theory, against effective parameters measured during steady state flow; (2) compare numerical simulation results based on the different formulations of effective parameters to measurements of transient events obtained in a two-dimensional laboratory experiment; and (3) analyze the performance of a deterministic two-dimensional model applied to a heterogeneous soil system by comparing numerical simulations to experimental data. The above analyses are carried out using data obtained from two-dimensional flow experiments in a 110 cm × 9 cm × 8 cm flow flume packed with well-defined heterogeneous sand configurations as discussed in detail by *Wildenschild and Jensen* [this issue].

2. Deterministic Modeling

First we analyzed the observed flow patterns in the heterogeneous laboratory system using the two-dimensional numerical flow model, SIM2D [*Gregersen*, 1995]. This model solves the Richards equation in two dimensions. The Galerkin finite element scheme based on triangular elements and linear interpolation functions is used to solve the time-independent part of the equation for each time step. The time derivatives are approximated by finite differences using a fully implicit approximation. Nonlinearities arising from the nonlinear water capacity and hydraulic conductivity functions are solved using Picard's iterative scheme. The time step is adjusted automatically during the simulation to ensure stability and fulfillment of mass balance. This same model will be used later for simulations using the effective parameters. In accordance with the physical experiment, the upper boundary condition for the simulations was a prescribed flux and the lower boundary was a prescribed suction, while no-flow boundaries were specified along the sides. A grid discretization of 5 cm in the horizontal direction and 1 cm in the vertical direction was used in the model. The porous plate was included in the model, and here a vertical discretization of 0.067 cm was used. The flow in the laboratory tank was at first simulated with identical *van Genuchten* [1980] (hereinafter referred to as VG) parameters (α and n) for both the retention and the hydraulic conductivity characteristics for each of the individual soil types (Table 1). The porosities were determined from the amount of sand packed in the pressure cell used for the retention curve measurement and the volume of the cell. Gravimetric tests following the experiments generally confirmed that the saturated water contents were virtually equal to the estimated porosity. The residual water content was estimated using a nonlinear least squares routine (RETC) by *Yates et al.* [1992], and the saturated hydraulic conductivity was measured in a long column experiment. We refer to *Wildenschild and Jensen* [this issue] for the details on the parameter estimation for the individual sands.

The model results did not match the observations very well using only one parameter set. Subsequently, independent sets of VG parameters (Table 1) were used for the retention and hydraulic conductivity functions leading to a much-improved

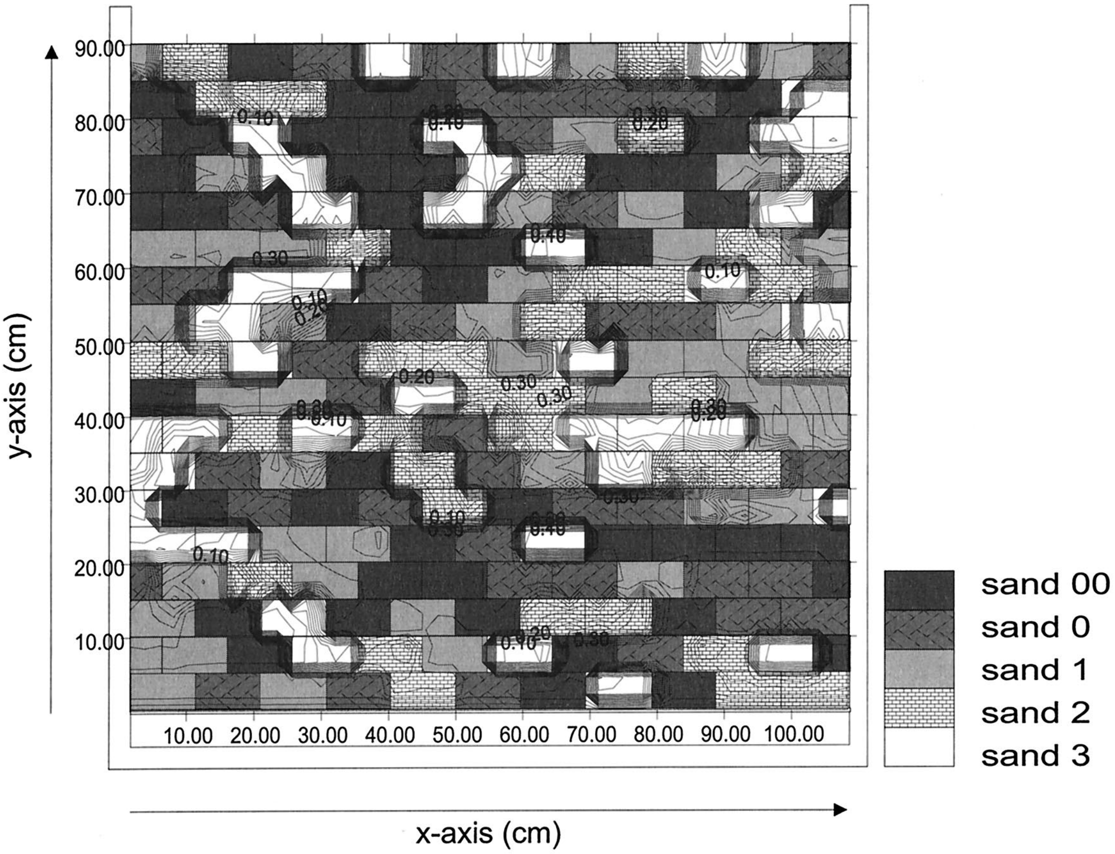

Figure 1. Simulated water content distribution in the tank at a steady flow rate of 1.6×10^{-5} m/s superimposed on the sand type distribution of the third experiment. Average volumetric water content measured at this flow rate was 0.19. Sand types vary between coarse (sand 3) and fine sand (sand 00).

match with the data, a result that suggests that one set of VG parameters may not always adequately describe variably saturated flow. However, using independent parameters is generally not an option for practical field problems since the unsaturated hydraulic conductivity characteristics are generally not measured.

Because of the presence of a suction boundary condition at the bottom of the tank, a uniform mean pressure distribution [*Wildenschild and Jensen*, this issue] prevails in the tank under steady state conditions. Figure 1 shows simulated distributions of the water content in the tank for a steady state situation where the applied Darcian flow rate was 1.6×10^{-5} m/s. Despite a relatively uniform mean pressure distribution, we observed considerable spatial variability in water content in the experiment (see also Figure 4), as an immediate result of differences in retention characteristics of the individual sands. Differences in water content between neighboring cells were simulated well by the deterministic model (Figure 1). Clearly, the finer sands retained much more water than the coarser sands at the prevailing suction. Some of the coarser grained sand cells had water contents close to the residual value, indicating that hardly any flow took place in these cells. Figure 2 illustrates the simulated flow paths through the tank under the flow conditions in Figure 1. Also, outlined in this figure are the flow patterns observed during a dye tracer experiment performed at the same steady state flow rate (see *Wildenschild and Jensen* [this issue] for details on the dye tracer experiment). The simulations show a highly tortuous pattern, consistent with the results of the dye tracer experiment. Figure 3 shows examples of simulated pressures along three different verticals ($x =$ 38.3, 78.3, and 98.3 cm) in the tank at two different flow rates (1.0×10^{-4} and 2.5×10^{-6} m/s). Also, shown in these figures are values measured with tensiometers in the same verticals (see *Wildenschild and Jensen* [this issue, Figure 2] for locations of tensiometers and time domain reflectometry (TDR) probes). The results show that the numerical model closely simulated the steady state pressure distributions measured in the tank. Some fluctuations in pressure were observed along the verticals, particularly at the lower flow rate. A similar phenomenon was reported by *Yeh* [1989] and *Yeh and Harvey* [1990] who observed that the fluctuations decreased with decreasing infiltration rate until a particular margin value was reached, thereafter they increased with decreasing infiltration rate. *Yeh* [1989] showed that even under these circumstances the use of the unit mean gradient approach was applicable, [see *Yeh*, 1989, Figure 9]. Agreement between simulated and measured water contents, however, was somewhat less favorable (Figure 4). A slight settling in the tank after packing and initial saturation may have caused some of the deviations. The settling observed in the tank for each individual layer was of a similar magnitude as the settling observed during the measurements on the individual sands (for instance pressure cell measurements). It was assumed that the impact of the settling on our analysis was of minor importance, except for the slight shift in vertical position of the tensiometers and TDR probes. Note that deviations are generally more noticeable for saturation

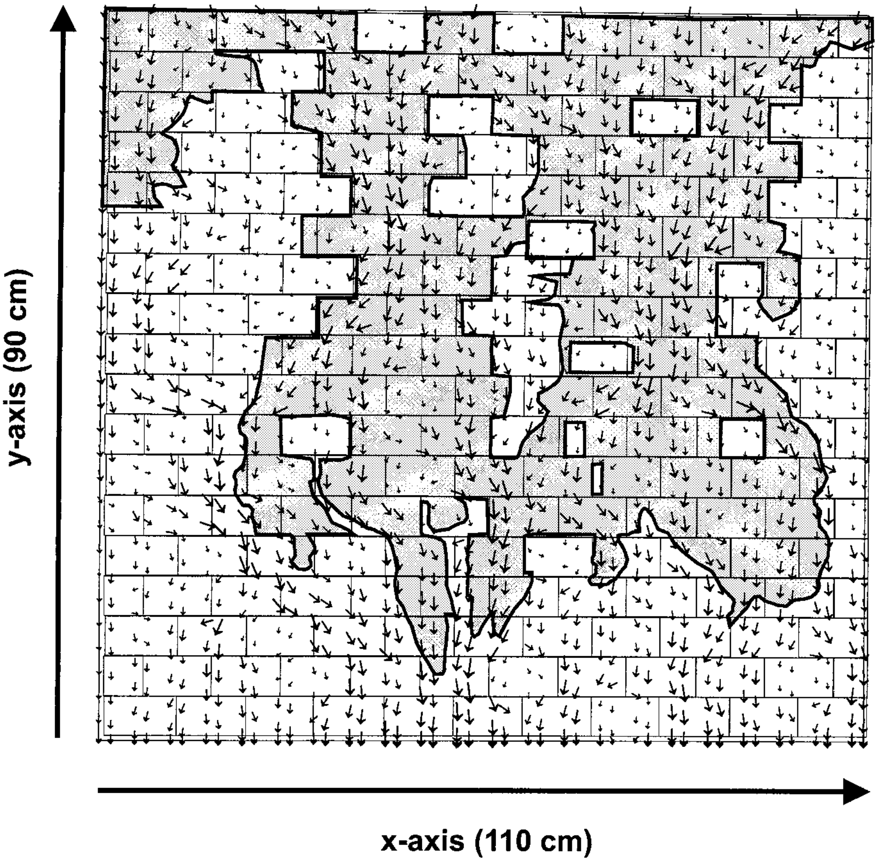

Figure 2. Flow pattern in the tank at a steady flow rate of 1.6 × 10^{-5} m/s observed during a dye tracer experiment (shaded area) and simulated using SIM2D (flow vectors) [*Gregersen*, 1995].

than for pressure, since the water content changes abruptly across cell boundaries.

The deterministic model was also used for simulating transient events monitored in the laboratory. Two examples of comparison between deterministically simulated and physically measured pressure changes are shown in Figure 5a and 6a. The deterministic model did not accurately match the average tensiometer readings in these examples (averaged at z position = 67.5 cm). Similar trends were observed when compared to averaged tensiometer readings at most other vertical positions in the tank. The values of the simulated pressures were generally too low, and the simulated transient pressure drops were too small. This last discrepancy is somewhat surprising since the individual tensiometer readings were matched quite well under steady state conditions. One could reason that averaging only five tensiometers at a particular level is not sufficient for deriving the average large-scale behavior. The five tensiometers at a given horizontal level could have been located in sand types that do not accurately represent in a statistical sense the tank as a whole (e.g., four coarse sand cells and one medium). The result may be biased readings caused by variations in capillary suction observed between the different sand types [cf. *Wildenschild and Jensen*, this issue, Table 3]. Differences between steady state and transient measurements of hydraulic properties as reported by, e.g., *Durner et al.* [1996], *Hollenbeck and Jensen* [1998], and *Plagge et al.* [1996] may also contribute to the observed discrepancies. Because of "dynamic nonequilibrium effects" or a rate-dependence of the hydraulic properties [*Hassanizadeh and Gray*, 1993], the properties describing static or steady state conditions may not adequately describe dynamic phenomena in the same medium. Air entrapment may be another source of error, as our model does not account for two-phase flow. The measured outflow rate, on the contrary, was simulated quite well using the deterministic approach (Figures 7a and 8a). This was not surprising since the physically measured outflow rate, by its very nature, is an average of the flow rates in the entire experimental tank. The two total discharge levels before and after changes in the flow rate should be simulated correctly unless the numerical model had a mass balance error. What is important is that the temporal variation during the flow rate changes was simulated very well also.

3. Identifying Effective Parameters

3.1. Measured Effective Properties: Case 1

The steady state measurements of the effective unsaturated hydraulic conductivity and retention characteristics were parameterized following the van Genuchten-Mualem expressions [*van Genuchten*, 1980; *Mualem*, 1976]. The resulting curves are shown in Figures 9 and 10, whereas the parameter estimates are listed in Table 1. The parameters, representing case 1 in Table 1, were estimated (by curve fitting) from the measurements of experiment number three because the modeling results presented here were based on the data from that experiment. The purpose of parameterizing these directly measured values of the effective hydraulic properties was to analyze whether they would also be useful for describing transient flow phenomena.

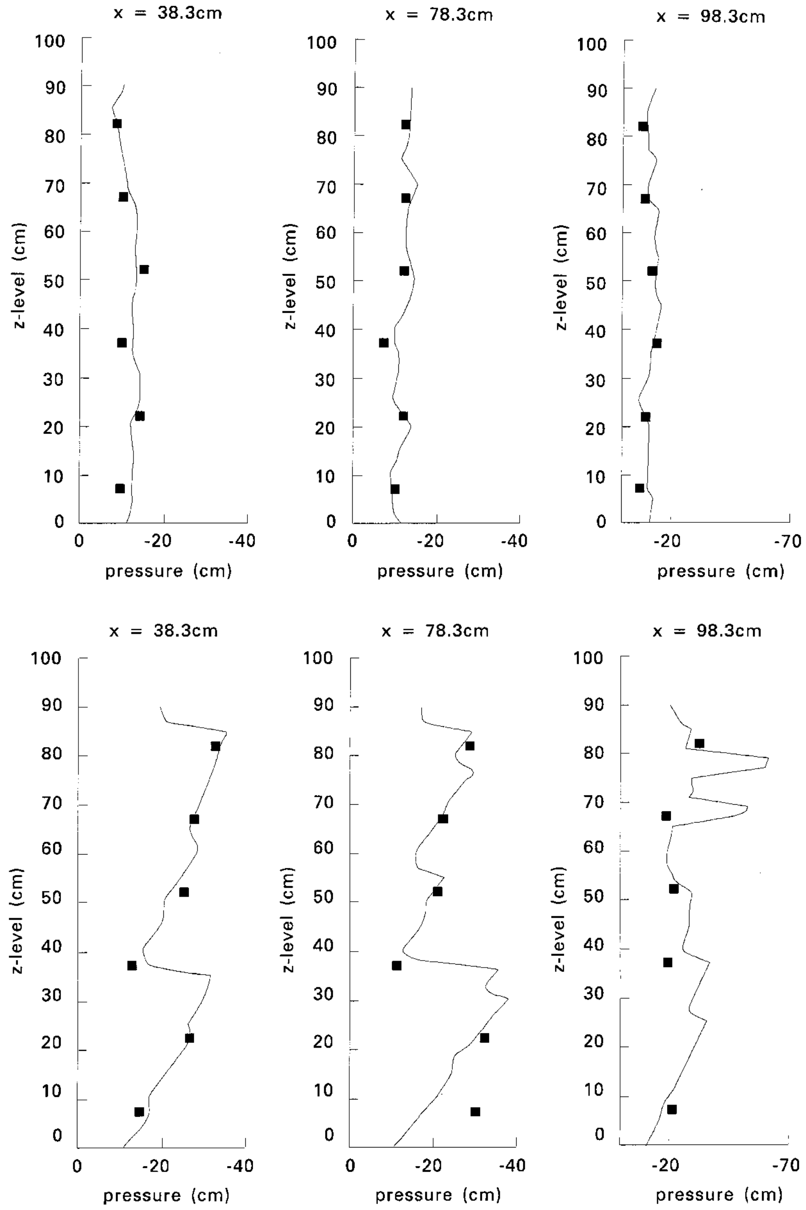

Figure 3. Simulated (lines) and observed (squares) vertical pressure distributions observed at three x locations at steady flow rates of (top) 1.0×10^{-4} m/s and (bottom) 2.5×10^{-6} m/s.

In addition to the effective properties derived form the direct measurements, seven other theoretical and empirical approaches to representing the effective hydraulic properties of the heterogeneous soil system were tested: case 2 inverse estimation from transient flow experiments, case 3 estimation using a stochastic model, where the effective hydraulic properties are derived from statistical characteristics of the local properties (homogeneous sands), and cases 4–8 using different, relatively simple, statistical averaging procedures on the local hydraulic properties of the homogeneous sands.

3.2. Inverse Estimates: Case 2

Inverse estimates of the effective parameters were obtained for some of the transient flow experiments performed on the tank. Steady state measurements of effective hydraulic properties were carried out at consecutive stages of steady state flow. Following each steady state situation, the applied flow rate was changed, and the resulting transient situation was monitored. Some of the transient events were used to inversely estimate the hydraulic parameters of the heterogeneous soil system using the nonlinear least squares optimization code SFIT [*Kool and Parker*, 1987]. Three consecutive changes in input flow rate were used for the optimization. Readings of the five tensiometers located 52.5 cm from the bottom of the tank (11–15) were averaged for each of the three steps in time for input to SFIT (see Figure 11). The optimization was performed on the tensiometer data only, while the stepwise changing flow rate was used as boundary condition. Thus the generally used objective function [see *Kool and Parker*, 1987] was reduced to

$$O(\mathbf{b}) = \sum_{i=1}^{N} \{V_i[\psi(t_i) - \psi_o(t_i, \mathbf{b})]\}^2 \qquad (1)$$

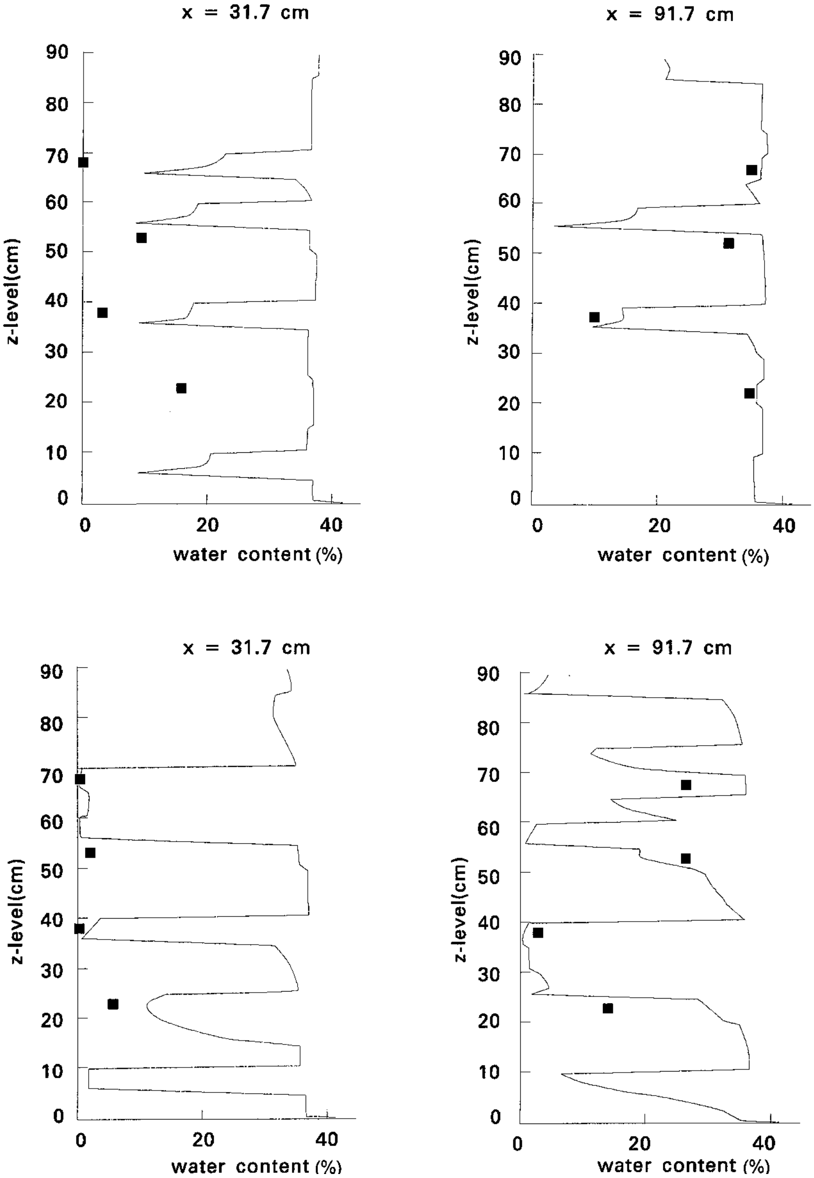

Figure 4. Simulated (lines) and observed (squares) water contents observed at two x locations at steady flow rates of (top) 1.0×10^{-4} m/s and (bottom) 2.5×10^{-6} m/s.

where **b** is a vector containing the optimized parameters, ψ is the measured capillary suction, ψ_o is the optimized suction, V is a weighting coefficient [*Kool and Parker*, 1987], and N is the number of measurements. We only optimized the VG parameters α and n. Including additional parameters in the optimization in most cases led to convergence problems. The remaining parameters were fixed at the values listed in Table 1. The optimization was considered unique when three different sets of initial estimates of α and n resulted in essentially identical optimized values of α and n. A regression coefficient of ~0.94 was obtained, while standard error coefficients were of the order of 0.5% for α and 1.3% for n. The optimized hydraulic conductivity and retention curves are shown in Figure 9 and 10, and the parameter estimates are listed in Table 1. Since SFIT handles only coupled retention and hydraulic conductivity parameters, the same α and n applies to the two hydraulic characteristic curves. The inversely estimated conductivity curve fit the measured data well, whereas the retention characteristic was less accurately represented. The fact that the inversely estimated hydraulic conductivity curve fits the measured curve quite satisfactory is rather encouraging because the experiments necessary to carry out the inverse approach are relatively simple and easy to execute. We only used average tensiometer readings (at one horizontal level) as input data in the present optimization.

3.3. Stochastic Approach: Case 3

The stochastic approach for large-scale transient unsaturated flow developed by *Mantoglou and Gelhar* [1987a, b, c] and *Mantoglou* [1992] considers the effects of three-dimensional flow and assumes that the local soil hydraulic properties are realizations of three-dimensional random fields. Under these circumstances a partial differential equation representing the large-scale flow conditions is derived; this equation is of the same form as the local governing flow equation and incorporates effective model parameters. The effective parameters entering the equation depend in a relatively complicated fashion on the statistical characteristics of the local soil properties [*Mantoglou and Gelhar*, 1987a, b, c].

The effective unsaturated hydraulic conductivity function for the heterogeneous laboratory tank was calculated using the stationary stochastic spectral approach discussed in detail by *Yeh et al.* [1985a, b, c], *Mantoglou and Gelhar* [1987a, b, c], and *Mantoglou* [1992]. With certain simplifying assumptions including that the mean flow is vertical and that the temporal changes in suction is small, *Mantoglou* [1992] developed the following

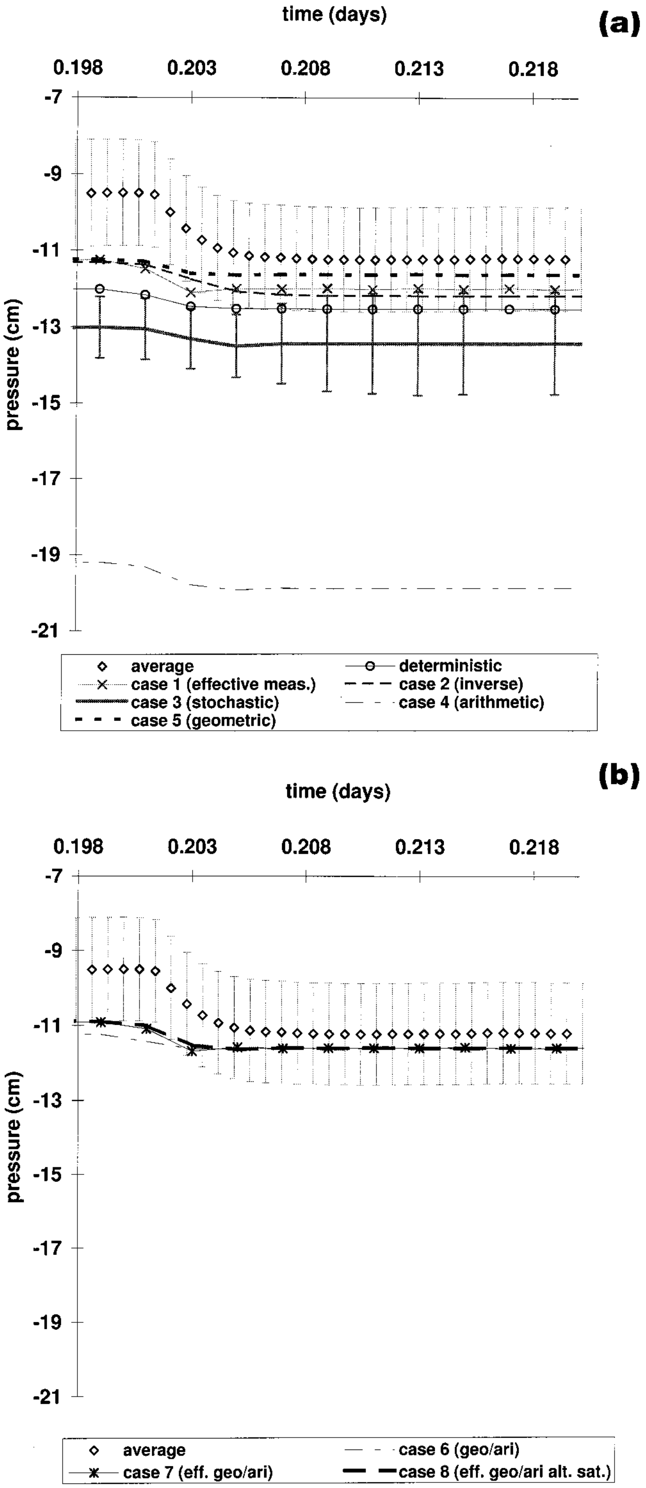

Figure 5. Simulated and measured capillary suctions for flow event 0914; $z = 67.5$ cm above the bottom of the tank. Vertical bars indicate standard deviations of the measurements (tensiometers 6–10). (a) Deterministic modeling and cases 1–5 and (b) cases 6–8.

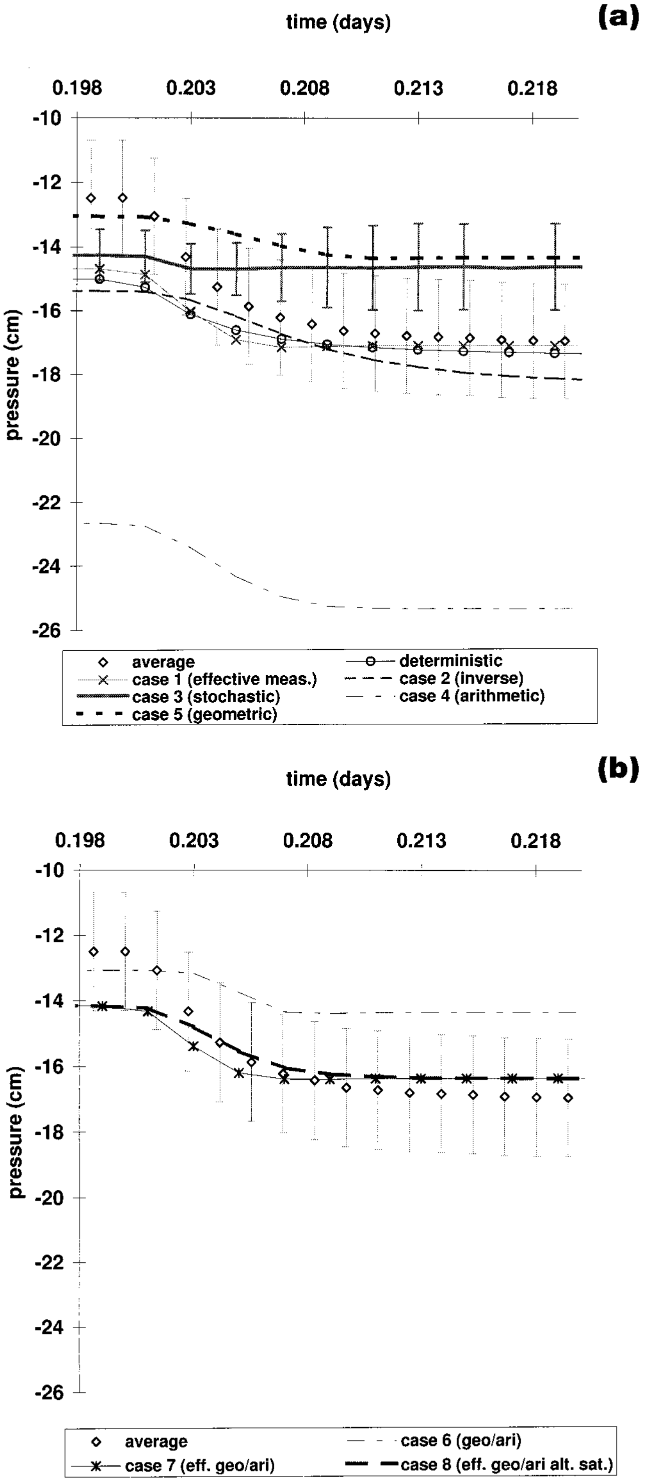

Figure 6. Simulated and measured capillary suctions for flow event 0917; $z = 67.5$ cm above the bottom of the tank. Vertical bars indicate standard deviations of the measurements (tensiometers 6–10). (a) Deterministic modeling and cases 1–5 and (b) cases 6–8.

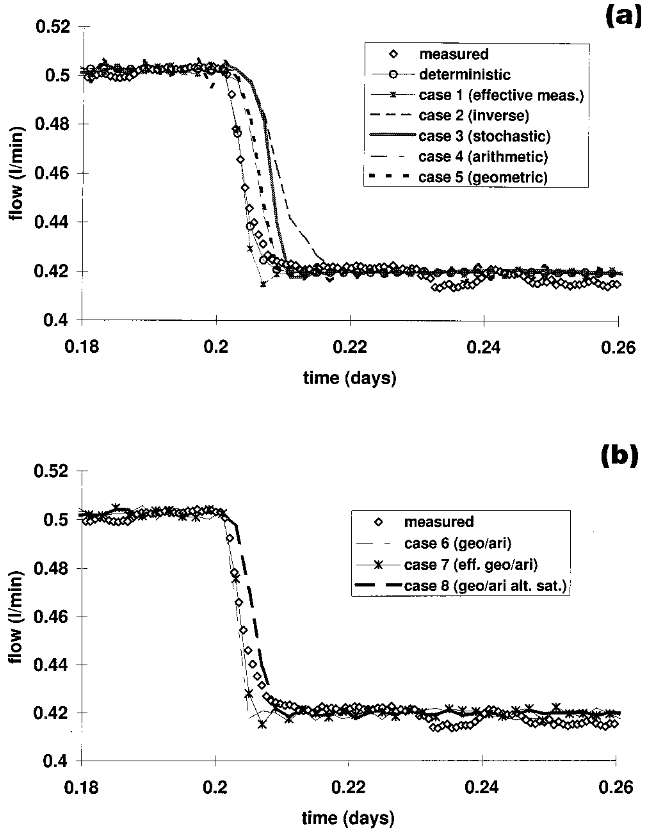

Figure 7. Simulated and measured outflow rates for flow event 0914. The flow rate is changed at $t = 0.2$ days. (a) Deterministic modeling and cases 1–5 and (b) cases 6–8.

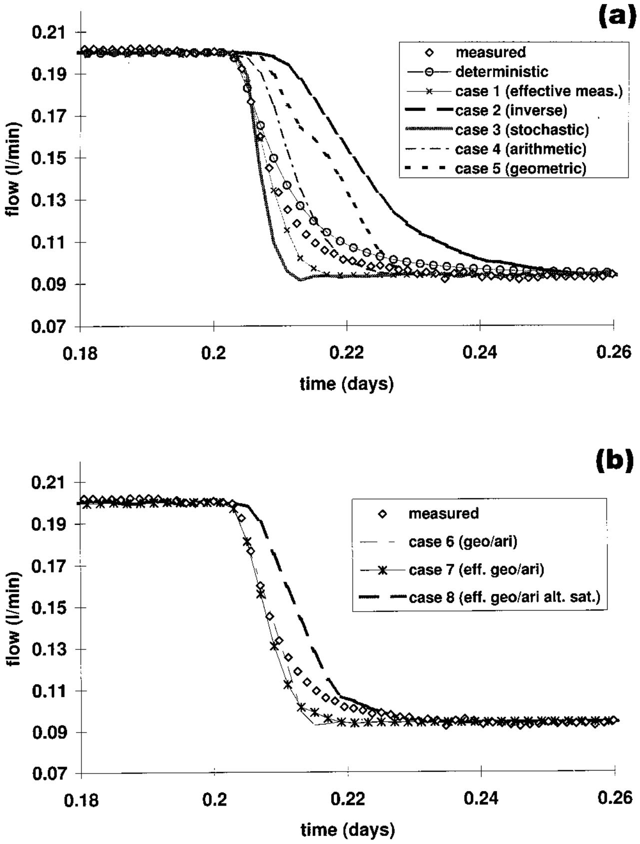

Figure 8. Simulated and measured outflow rates for flow event 0917. The flow rate is changed at $t = 0.2$ days. (a) Deterministic modeling and cases 1–5 and (b) cases 6–8.

expressions for the vertical effective hydraulic conductivity for an isotropic soil:

$$K_{\mathrm{eff}}(H) = e^{Y(H)} \exp\left\{ -\sigma_y^2\left[\frac{C_{ya}}{A\sigma_y^2}+\frac{2}{r}-\frac{4}{r^2}+\left(\frac{C_{ya}}{A\sigma_y^2}-\frac{1}{2}\right)\frac{1}{1+r} + \left(\frac{4}{r^3}-\frac{1}{r}-\frac{2}{r}\frac{C_{ya}}{A\sigma_y^2}\right)\ln(1+r)\right]\right\} \qquad (2)$$

where K_{eff} is the vertical effective unsaturated hydraulic conductivity, H is the mean suction head, and $r = AL_{1\gamma}$ in which A is the mean of the slope of the local hydraulic conductivity curve, $L_1 = J_1 + \partial H/\partial z$ and J_1 is the mean head gradient, and γ is the isotropic correlation length. $Y(H)$ and σ_y^2 in (2) are the mean and variance of the natural logarithm of the local hydraulic conductivity, respectively, while C_{ya} is the correlation between y and a. The variance of the predicted suction ψ (model error) is in this case given by

$$\sigma_\psi^2 = \sigma_y^2\lambda^2 J_1^2\left[-\frac{1}{r}+\frac{2}{r^2}+\frac{1}{1+r}-\frac{2}{r^3}\ln(1+r)\right] \qquad (3)$$

For the same assumptions, *Mantoglou* [1992] also derived an expression for vertical $K_{\mathrm{eff}}(H)$ for a stratified soil:

$$K_{\mathrm{eff}}(H) = e^{Y(H)} \exp\left[-\frac{\sigma_y^2 + 2C_{ya}\gamma_1 J_1}{2(1+AL_1\gamma_1)}\right] \qquad (4)$$

where the parameters are defined as above and γ_1 is the vertical correlation length. The variance of ψ in this case is given by

$$\sigma_\psi^2 = \frac{\sigma_y^2\lambda_1 J_1^2}{AL_1(1+AL_1\lambda_1)} \qquad (5)$$

In view of discussions by *Mantoglou and Gelhar* [1987b] and the example of *Jensen and Mantoglou* [1992], the effective specific water capacity (C_{eff}) in our study was derived from the

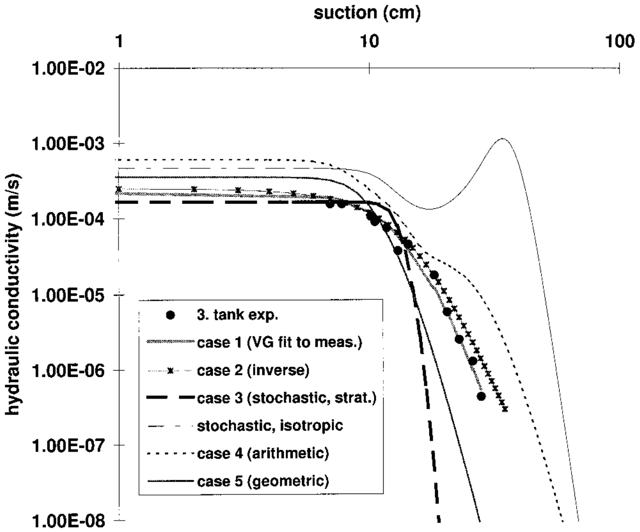

Figure 9. Comparison of measured and estimated effective unsaturated hydraulic conductivity characteristics.

geometric average of the individual retention characteristics, instead of using the stochastic representation. This approach is possible since the effect of variability of this parameter on the system mean hydraulic behavior has been shown to be of less importance compared to the effect of variability of the hydraulic conductivity.

The statistical parameters required by the stochastic model were derived from knowledge of the functional representations of the local retention and hydraulic conductivity curves. We refer to *Mantoglou and Gelhar* [1987a, b, c] and *Mantoglou* [1992] for the details of the estimation of the various parameters used in this approach. The correlation lengths γ and γ_1 were approximated by the length of the individual heterogeneities (10 cm). The mean head gradient J_1 was assumed to be unity, and the gradient $\partial H/\partial z$ was set to zero, leading to $L_1 = 1$. Since the heterogeneous soil system investigated in our study was structured somewhere between the isotropic and stratified cases, we chose to apply both (2) and (4). Ideally, the heterogeneous system should be considered isotropic, but since some of the sand types were replicated several times in neighboring grid cells, flow conditions in the tank may have resembled, in a few cases, those expected in a stratified system.

The resulting effective unsaturated hydraulic conductivity functions for both the isotropic and the stratified assumption are shown in Figure 9. The stratified approach represents the measured conductivities relatively well, while the isotropic approach deviates considerably. The unrealistic shape of the isotropic curve is mainly caused by a large variation in the natural log of the hydraulic conductivity. The natural log of the K variance dominates the expression for the effective conductivity in the isotropic case and causes the relatively large deviation from the experimental data. The first-order perturbation approach has been shown to be robust for relatively large variances in the input hydraulic conductivity [*Gelhar*, 1986]. However, the variance in ln (K) is in our case between 1 and 2 orders of magnitude greater than what *Gelhar* [1986] considers a serious violation of the stochastic theory. This fact makes the use of stochastic theory for our heterogeneous soil system questionable. As a consequence of the unrealistic shape of the isotropic curve, only the stratified case will be further considered when modeling the transient flow scenarios.

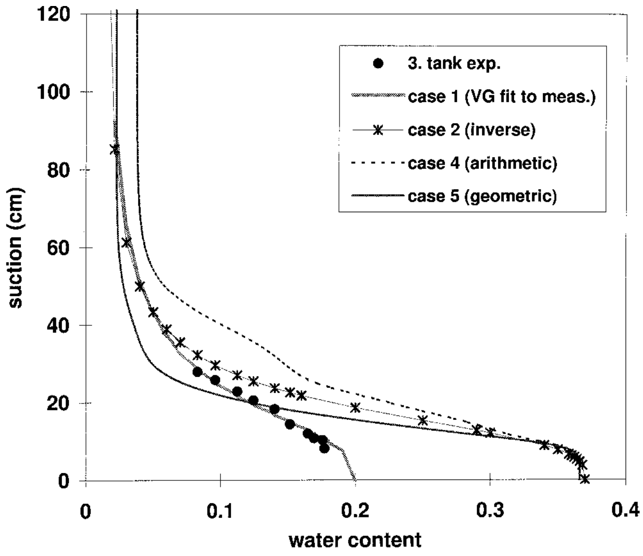

Figure 10. Comparison of measured and estimated effective retention characteristics.

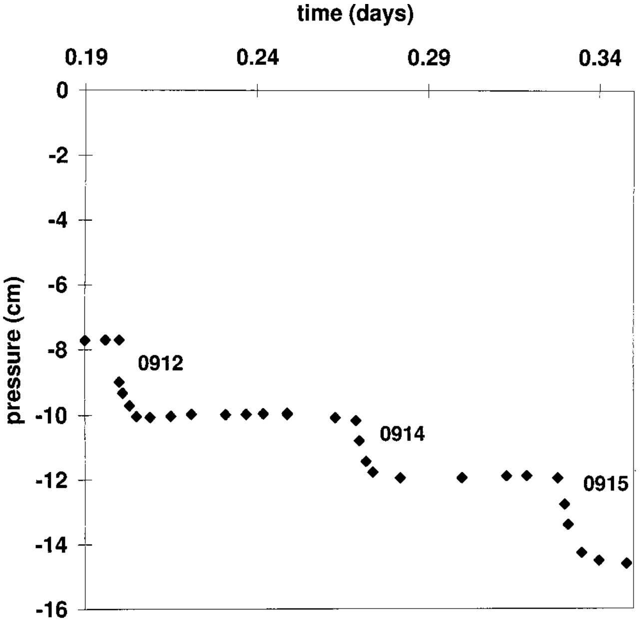

Figure 11. Transient pressure measurements used in the inverse estimation. Pressures are averages of five tensiometers located at 52.5 cm from the bottom of the tank (tensiometer 11–15).

3.4. Direct Averaging Approaches: Cases 4–8

We now address the issue of whether it is possible to represent the effective hydraulic properties of a heterogeneous system as some average of the properties of its component parts. Arguments have been made that averaging of the hydraulic properties is not valid because of the nonlinear behavior of unsaturated flow [*Yeh et al.*, 1985c; *Ferrand and Celia*, 1992]. While this argument may be formally correct, a direct averaging may still prove useful to provide rough estimates when relatively simple soil systems are considered. We derived effective hydraulic conductivity and retention curves by both arithmetic (case 4) and geometric (case 5) averaging. The arithmetic and geometric curves were obtained using the following procedure: VG parameters were fitted to the measured curves of the individual sands (parameters listed in Table 1) and continuous curves established based on these estimates. Subsequently, hydraulic conductivity and water content values were determined as weighted (by percent of each sand type in the laboratory tank) arithmetic or geometric averages at consecutive suction values, and the resulting curves were parameterized (Table 1). This approach was chosen instead of statistical averages of the VG parameters, which, because of the nonlinearity of the parametric models, would have resulted in biased curves [*Green et al.*, 1996]. The resulting unsaturated hydraulic conductivity and soil water retention curves are shown and compared with the directly measured values in Figures 9 and 10, respectively. The agreement between the geometrically averaged retention curve and the measured values is acceptable as both the level of the air entry pressure and the slope of the curve seem to be fairly well represented. The slope of the arithmetic retention curve, however, is overestimated, although the air entry level is similar to that of the geometric curve. The arithmetically averaged hydraulic con-

Table 2. Transient Flow Events Used for Evaluation of the Different Simulation Approaches

Flow Event	Initial Flow Rate, m/s	Final Flow Rate, m/s
0912	1.6 10^{-4}	1.24 10^{-4}
0914	9.5 10^{-5}	8.0 10^{-5}
0915	7.4 10^{-5}	4.7 10^{-5}
0917	3.8 10^{-5}	1.8 10^{-5}

ductivity curve overestimated the measured hydraulic conductivity at a given suction, particularly at the higher values, whereas the geometric curve to some degree underestimated the hydraulic conductivity. The general shape of the geometric curve matched the measurements better than the arithmetic function. *Yeh and Harvey* [1990] obtained similar results for both drying and wetting hydraulic conductivity curves. The mathematical definitions of the two averages implies that the geometric average value will always be lower than the arithmetic curve but not necessarily always at the same distance from each other.

Three alternative averaging schemes were introduced to possibly further improve the match between the transient simulations and the measurements. These additional approaches are based on combinations of the previously discussed arithmetically and geometrically averaged data and therefore not further discussed in relation to the steady state measurements. Figure 9 shows that the best match to the directly measured unsaturated hydraulic conductivity characteristics was obtained with the inverse approach. This result was not surprising because contrary to the other approaches, which are based on statistical information of the hydraulic properties of the individual sands, the inverse approach is based on experimental data that convey explicit information about the combined heterogeneous system behavior, and the approach hence should result in more representative parameter estimates. The geometric and stochastic stratified approaches appear to be acceptable, while the arithmetic and stochastic isotropic approaches are far less convincing. The stratified approach slightly underestimated the hydraulic conductivity, reflecting the fact that flow in a stratified soil tends to be hampered by layers of low conductivity which causes the overall flow rate to decrease. The opposite situation is true for the isotropic case where water can move freely around cells of lower conductivity. Since our system behaves between these two extremes, it is intuitively apparent that the laboratory measurements are located between the two stochastic estimates.

4. Numerical Modeling Transient Conditions

The first part of this study demonstrated that there are several ways to estimate the effective hydraulic parameters for a heterogeneous soil system, with some of these approaches being more practical than others. For instance, direct measurement of the effective parameters is not an option when actual field-scale problems are considered in a predictive mode, since data acquisition for such an approach would be an impossible task. Also, approaches that work well for steady state conditions may not perform equally well during transient flow. The issue of applicability of steady state measurements in heterogeneous systems was also a concern of *Smith and Dirkkrüger* [1996], who stated in their concluding remarks that hydraulic characteristics measured on a heterogeneous sample (whatever the scale) cannot be used to describe unsteady flows through that sample.

Thus, to evaluate the performance of the different steady state derived effective parameter estimates, they were used as equivalent homogeneous parameters representing the heterogeneous system in a deterministic numerical model and compared to transient measurements of mean capillary suction and outflow rate monitored in the laboratory experiments.

As mentioned previously, we used the SIM2D code of *Gregersen* [1995] to simulate the experiments. Instead of using a distributed description of the soil system as in the deterministic simulations, the heterogeneous tank was now represented by various estimates of effective values of the hydraulic parameters, and the problems were solved in only one dimension. A slightly larger discretization was used for these one-dimensional simulations with node distances varying between 0.067 cm in the porous plate and increasing to a maximum of ~3 cm in the bulk soil. This increased discretization was verified to produce identical results as compared to simulations carried out with a discretization of ~1 cm. Solutions were obtained for two sets of parameter values representing retention and hydraulic conductivity characteristics separately, except for the inverse approach where only one set of parameter values was estimated. Four different events monitored in the laboratory were simulated representing transient changes from one steady state flow rate to another (Table 2). The rate referred to as "initial flow rate" was maintained for 0.2 days and then instantly changed to the "final flow rate." The results of the simulations are shown in Figures 5–8 for two events (0914 and 0917). Figures 5 and 6 show simulated pressures for the different approaches following the change in input flow rate, as well as the measured response of the average pressure readings of five tensiometers (6–10) located 67.5 cm above the bottom of the tank. Figures 7 and 8 show the corresponding measured and simulated transient change in flow rate measured at the outlet of the tank. In addition to the qualitative comparison of observations and simulations shown in the figures, Table 3 lists the root-mean-square-error (RMSE) coefficients of the differences between observations and simulations at the discrete times shown in Figures 5–8 for the various approaches. These coefficients represent a quantitative measure that in conjunction with the figures can assist in evaluating the accuracy of the various approaches.

4.1. Suction Measurements

Simulations of the average pressure using arithmetically averaged hydraulic properties underestimated the values measured at $z = 67.5$ cm for both flow events shown in Figures 5a and 6a. The simulations deviated by 8–10 cm, which is approximately the magnitude of the measurements; in neither event are they within the range of the standard deviation of the measurements. Simulations using the geometric averages were much closer to the measured suctions as also reflected in the RMSE coefficients listed in Table 3. The simulations still deviated somewhat from the measurements, but they were within the range of the standard deviations of the measurements for both events. A similar good agreement was obtained for the simulations based on the effective parameters derived from the directly measured data and for the inverse estimates. These last two approaches appear to be slightly better at the lower pressure (lower flow rate) as illustrated in Figure 6a. Note that the optimization of the inverse estimates was based on aver-

Table 3. Root-Mean-Square-Error Coefficients for the Differences Between Observations and Simulations

	Deterministic	Eff. Meas. (Case 1)	Inverse (Case 2)	Stochastic (Case 3)	Arith. (Case 4)	Geom. (Case 5)	Geom./Arith. (Case 6)	Eff. Geom./Arith. (Case 7)	Eff. Geom./Arith. Alt. Sat. (Case 8)
0914 pressure (Figure 5)	1.7365	1.1718	1.2238	2.6687	9.3636	0.9093	0.9391	0.8127	0.7797
0917 pressure (Figure 6)	1.2851	1.1653	1.4731	1.9291	9.2916	2.2132	2.1617	0.8336	0.7745
0914 flow (Figure 7)	0.0037	0.0077	0.0283	0.0246	0.0121	0.0146	0.0110	0.0080	0.0106
0917 flow (Figure 8)	0.0096	0.0081	0.0534	0.0168	0.0212	0.0403	0.0089	0.0079	0.0239

RMSE = $[1/(n-1)\ \Sigma_{i=1}^{n}\ (p_i - p_o)^2]^{1/2}$, where p_i is either pressure or flow simulation and p_o is the measured value of pressure or flow; N is the number of data points used in the calculation of the RMSE. Alt. Sat., alternate saturation.

ages of tensiometers 11–15, while the average readings of five different tensiometers 6–10 (different level in the tank) were used in the comparison. The stochastic stratified approach deviated at the higher flow rate (0914) but was still within 1 s.d. at the lower flow rate (0917). One of the merits of the stochastic theory is that expressions for the model error of the predictions (pressure variance) can be derived (Equation (5)). The standard errors as calculated from this expression were generally between 5 and 10% of the simulated mean values. Generally, the numerical simulations did not accurately reproduce the relatively quick pressure drops measured with the tensiometers following changes in the flow rate. Most of the simulations also deviate somewhat with respect to the pressure level. Even the deterministic simulations are unable to produce the abrupt change in pressure observed in the laboratory. As reasoned earlier, the small number of tensiometers used in the comparisons could have contributed to the discrepancies; however, this does not explain the insufficient responses in simulated pressure changes. In an attempt to improve the agreement between measured and simulated pressures and outflow rates, several alternative approaches (cases 6–8) were tested. Case 6 employs a combination of arithmetically averaged retention data and geometrically averaged hydraulic conductivity data of the individual (local) sands. That means that the parameters listed in Table 1 for case 4 are used in the numerical model when retention is considered and the parameters listed under case 5 in Table 1 are used for hydraulic conductivity calculations. The incentive for this type of averaging is the fact that the conductivity is generally lognormally distributed, while the retention data are more likely to be normally distributed, at least for not too broad a suction interval. Case 7 is also a combination of arithmetically averaged retention data and geometrically averaged hydraulic conductivity data, except that now averages of the effective parameters derived from the direct measurements (not the individual sands) are used. In other words, arithmetic averages of the 30 tensiometers are combined with the arithmetic average of the 12 TDR probes, and geometric averages of the 30 tensiometers are combined with the flow measurements. Finally, case 8 is identical to case 7 except that θ_s is fixed at its calculated saturated water content (0.366) rather than using the fitted value of $\theta_s = 0.200$. The capillary suctions simulated using these alternative approaches are presented in Figure 5b and 6b. The use of the combined arithmetic/geometric averages of the local data (case 6) resulted in capillary suctions that are almost identical to the ones obtained with the geometric averages (case 5) (see also Table 3). The match was improved at both flow rates when using the combined arithmetic/geometric averages of the measured effective values (cases 7 and 8) relative to case 1. Using the higher saturated water content (case 8) did not yield significantly different results.

4.2. Flow Measurements

The measured and simulated responses in the outflow rate are shown in Figures 7 and 8 for the two flow rates discussed in this study (0914 and 0917). As was the case for the suction measurements, the measured effective hydraulic properties (case 1) yielded relatively good results. The inverse approach, however, did not result in good comparisons between measurements and simulations. The outflow response to the change in flow rate is too slow as compared to the measurements, with the deviations becoming quite large at the lower flow rates. These deviations could to some degree be expected since the inverse estimates were obtained solely on the basis of tensiometer readings. Improvements could probably be achieved by incorporating variables in the optimization that represent a greater variety of flow characteristics, such as measured outflow rates and water contents.

The arithmetic and geometric averages also resulted in flow rate responses that were too slow. The simulated flow rates obtained with these two approaches are very close at the higher flow rate (Figure 7a), while the arithmetic average simulations are better, but certainly not satisfactory, at the lower flow rate (Figure 8a). Geometrically averaged estimates underpredicted the hydraulic conductivity at steady state (Figure 9), which means a slower response at the outlet as was also observed in Figure 8a.

Outflow simulations obtained with the stochastic approach did not perform well at the high flow rate (close to saturation) as shown in Figure 7a, probably due to the fact that $A(H)$ and C_{ya} in K_{eff} for the stratified case (equation (4)) are very close to zero for pressures close to zero. However, the performance of the stochastic estimate improves with decreasing pressure (Figure 8a), a trend that was also noted in other simulations not discussed here.

The simulated responses to the transient change in flow rate were generally too slow. This effect was found to increase with decreasing flow rate (decreasing pressure). The measured rapid response to changes in the flow rate is likely an effect of the spatial variability of the hydraulic properties in the heterogeneous tank. Differences in conductivity between the different sands become more pronounced with increasing suction, which causes flow to be confined to increasingly more restricted parts of the tank, thus leading to more pronounced

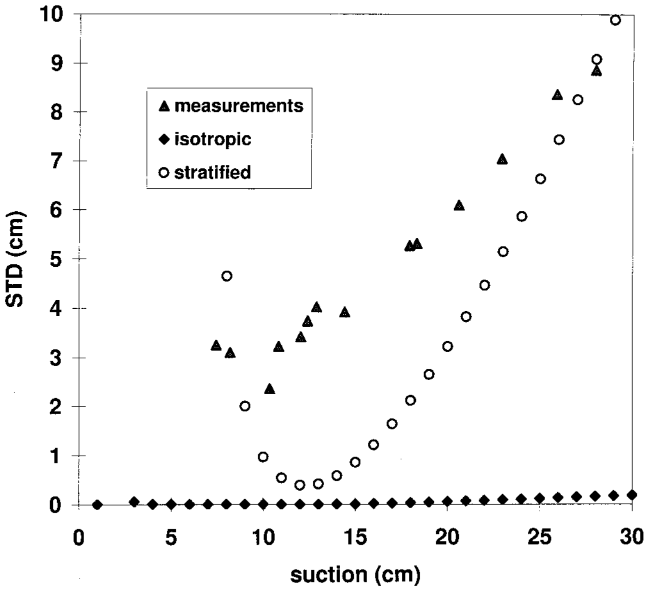

Figure 12. Measured and estimated (using stochastic theory) capillary suction variances as a function of their mean values.

preferential flow. Simulations based on the stochastic theory (and of course the deterministic simulations) are better capable of considering the effects of heterogeneity and hence should predict the fast response observed in the experiments better. The same is true for the simulations using the measured effective properties, which directly account for the spatial variability of the tank.

The alternative approaches using combined arithmetic/geometric averages resulted in improved simulations of the outflow response. The response time was notably improved at both flow rates in Figures 7b and 8b. Even the combined arithmetic/geometric averages based on the local values (case 6) produced faster responses. Apparently, the combination of the arithmetic and geometric averages of the hydraulic properties has more influence on the (dynamic) hydraulic conductivity (i.e., flow rate) than on the static properties of the retention curve. Analogous to the simulated capillary suctions, simulations of the measured outflow rate did not improve when using a higher saturated water content (case 8); actually, the opposite was found to be the case. The response to changes in outflow rate was delayed in the case of higher saturated water content. One possible explanation could be that preferential flow due to differences in water content among individual cells would be less dominant if a higher water content prevails in the tank. Another possible reason for the slower response could be the greater storage available in the tank if the porosity is higher.

As was the case for the pressure measurements, deviations between simulated and measured outflow rates were generally increasing with decreasing pressure (increasing capillary suction) corresponding to increased effect of heterogeneity. This phenomenon is also illustrated in Figure 12, which shows calculated (based on stochastic theory) and measured capillary suction variances obtained at steady state as a function of their mean value. A distinct increase in variance with mean capillary suction was observed for both the laboratory measurements, and the theoretical values based on the stochastic stratified theory. These results corroborate the findings of *Yeh and Harvey* [1990]. The latter relationship had a somewhat different shape than the measurements but was within the same range. By comparison, the isotropic curve did not match the measurements very well.

5. Conclusions

Different effective hydraulic parameter estimates based on either simple statistical averages of the local properties, inverse estimates derived from transient experiments, or the more involved stochastic theories were established and compared to measurements obtained in a two-dimensional tank experiment. The inverse, geometric average, and stochastic (stratified) approaches matched the steady state measurements of the hydraulic characteristics quite well. Deterministic modeling of steady state scenarios verified the performance of the traditional approach when hydraulic properties and boundary conditions are well defined, in which case the simulations and measurements matched well.

The different parameter estimates were used for modeling transient flow scenarios observed in the laboratory. In addition to the theoretically/empirically obtained estimates, the measured effective hydraulic properties were also used in these simulations. In general, the values of the capillary suction measurements were simulated in an acceptable way using the different approaches, except when the arithmetic average was employed. However, most of the numerical simulations (including the deterministic approach) did not accurately reproduce the relatively quick pressure drops measured with the tensiometers following changes in the flow rate. Transient changes in the outflow rate were not described in an entirely satisfying fashion using the different simulations either. Simulated responses were generally too slow as compared to the measurements. Exceptions were the deterministic approach and simulations based on "effective" parameters derived from the direct measurements, which both performed quite well, the latter case suggesting that the concept of effective parameters is valid. Unfortunately, these two approaches are not a practical option when field-scale problems are considered.

A combination of arithmetical (retention) and geometrical (hydraulic conductivity) averaging of the local hydraulic properties produced outflow responses that compared very well to the measurements. However, similar satisfactory agreement was not obtained between simulated and measured capillary suctions.

The stochastic approach generally also predicted fast changes in the outflow rate. Of the more successful approaches, the stochastic model was the only one capable of incorporating the effects of spatial variability in soil hydraulic properties on the average system behavior in a physically plausible manner, and, as an important feature, it offers a framework for assessing the uncertainty of the predicted mean behavior and therefore deserves attention in future investigations. Inverse procedures may also prove to be advantageous in future investigations, despite their less than optimal performance in our studies. Experiments for the optimization are often quite easy to carry out, while the information retrieved may be more representative of the heterogeneous soil system being studied.

Finally, we would like to emphasize that the results reported in this study were obtained for very specialized heterogeneous configurations. These configurations were constructed of block units of well-sorted sands of known hydraulic properties, configurations that may not be particularly representative of field conditions. We believe that our experiments constitute an important intermediate step toward obtaining a better process understanding and an improved insight into the applicability of the concept of effective parameters for heterogeneous soils because of the improved experimental control that can be obtained in the laboratory in comparison to a field experiment. For the system and flow conditions investigated in this study, it was shown that it was possible to identify effective hydraulic properties and that these properties could be used to represent the heterogeneous medium in numerical model simulations. At the same time we recognize that our systems were synthetic and that there is need for validation of our results before applying them to a different type of heterogeneous system.

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