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Vadose Zone Transport Field Study FY 2001 Status Report: Determination of Field-Scale Hydraulic Parameters by Inverse Modeling

Z. F. Zhang
A. L. Ward
G. W. Gee

October 2001

Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RL01830

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Richland, Washington 99352

Summary

There is an urgent need for more information about the transport of contaminants as they move through the vadose zone to the underlying water table at the Hanford Site near Richland, Washington. This document describes a conceptual model to characterize the soil hydraulic properties of the Hanford Site. Preliminary tests of the model have been conducted.

The accurate prediction of water flow and contaminant transport in unsaturated porous media is hampered by insufficient and uncertain constitutive property information. We proposed a non-similar media scaling method that can be coupled with inverse flow modeling to estimate constitutive parameters for heterogeneous soils. By assigning the scaling factors to the same soil layers in the field, the reference hydraulic parameter values at field scale can be estimated through inverse modeling of well-designed field experiments. Parameters for individual layers are then obtained through inverse scaling of the reference values using the *a priori* relationships between the reference parameter values and the specific value for each layer.

The numerical simulator, STOMP, was combined with the inverse modeling program, UCODE, to estimate the hydraulic parameters. Three cases of soil heterogeneity, i.e., homogeneous soil, layered soil, and heterogeneous soil, were considered. For the drainage experiment in the North Caisson with homogeneous soil near the Buried Wastes Test Facility, soil-water contents (θ) were overestimated, and most of the pressure heads (ψ) were underestimated when the lab-scale parameter values were used. When the field-scale parameter values were used, both θ and ψ were well predicted. For the drainage experiment in the Grass Site with layered soil, both soil-water contents and pressure head were significantly overestimated when the local-scale parameter values were used. When the field-scale parameter estimates obtained by the inverse method were used to predict the flow, the prediction errors were much smaller than those using the local-scale parameter values. The slopes of the trend lines between the observed and predicted values were 0.956 to 0.997 for θ and ψ, respectively. Preliminary work has been conducted to estimate the hydraulic parameters of a small section of the Sisson and Lu site in the 200East area. When the lab-scale parameter values were used to predict water contents, there was a very low correlation between the predictions and observations ($R^2 = 0.28$). This correlation was significantly improved ($R^2 = 0.74$) when the inversely estimated field-scale parameter values were used. The standard deviation was 0.0175 m^3m^{-3}, and the 95% linear confidence interval was ± 0.034 m^3m^{-3}.

Glossary

3-D	three dimensional
BWTF	Buried Wastes Test Facility
CI	confidence interval
CPU	central processing unit
CSS	composite scaled sensitivities
HYDRUSS	????????????
LCI	linear confidence interval
NSM	non-similar media
PNNL	Pacific Northwest National Laboratory
STOMP	Subsurface Transport Over Multiple Phases
SUFI	sequential uncertainty domain parameter fitting
UCODE	Universal CODE

Acknowledgments

We thank Mark White for his help in implementing the modifications to STOMP and Eileen Poeter of the Colorado School of Mines for fixing a couple of bugs discovered in the application of UCODE to the unsaturated flow problems. Pacific Northwest National Laboratory is operated for the U.S. Department of Energy under Contract DE-AC06-76RL01830.

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1.0 Introduction

Many laboratory methods exist to determine the highly nonlinear soil-hydraulic functions represented by the soil-water retention and unsaturated hydraulic conductivity curves (e.g., Klute and Dirksen 1986; Klute 1986). However, laboratory-determined parameters are usually not applicable to real field situations (e.g., Wierenga et al. 1991). The inverse procedure uses the nonlinear regression method to estimate hydraulic parameters. The method requires the minimization of differences between measured dependent variables and appropriate analytical or numerical solutions that contain the set of parameters to be estimated. A number of laboratory and field applications (van Dam et al. 1992; Parkin et al. 1995; Simunek and van Genuchten 1996; Lehmann and Ackerer 1997; Abbaspour et al. 1997; Inoue et al. 2000; Zhang et al. 2000) have shown the great potential of the inverse technique for improving the designs and analyses of vadose-zone flow and transport experiments. Kool et al. (1987) and Hopmans and Simunek (1999) reviewed inverse techniques to estimate flow and transport parameters.

However, determination of the soil hydraulic parameters of layered soils using the inverse procedure remains a challenge. Abbaspour et al. (1997) proposed a sequential uncertainty domain parameter fitting (SUFI) procedure to inversely estimate soil hydraulic parameters. Abbaspour et al. (2000) linked SUFI with the one-dimensional flow model HYDRUS5 to estimate up to 32 hydraulic parameters of a four-layer soil. They found that fitting alone, even with 20 to 30 parameters, could not account satisfactorily for the soil hydraulic behavior. Rather, correct accounting of the soil hydraulic processes as well as the soil system proved to be essential.

When more parameters are estimated using the inverse method, the inverse model becomes more difficult to converge or converges to local minima in the multi-dimensional parameter system. The problem becomes very complex when the number of parameters to be estimated becomes large (e.g., more than 10). Further, the inverse modeling is very central processing unit (CPU) intensive when the number of parameters to be estimated is large. To minimize the difficulty and cost of characterizing water flow through heterogeneous field soils, scaling approaches have evolved in an attempt to reduce the number of hydraulic parameters needed. Shouse et al. (1992) applied the scaling of water content to vertically heterogeneous soils by allowing the scale factors to vary with depth. Then they estimated the unsaturated hydraulic functions based on the scaled flow equation. They found that scaling θ successfully coalesced heterogeneous soil hydraulic properties into unique functions for both $\theta(\psi)$ and $K(\theta)$. Warrick (1993) used the inverse method to estimate soil hydraulic parameters based on the scaled Richards' equation. First, transient experimental data of the cumulative infiltration rate were optimized using Philip's (1969) quasi-analytical, algebraic forms. Then the results of Warrick et al. (1985) that were based on the similar media scaling (Miller and Miller 1956) were used to find properties that match the fitted results.

Vogel et al. (1991) introduced the linear-variability concept that expresses the soil hydraulic properties in terms of a linear transformation. They extended the similar-media concept by introducing three scaling factors, which are associated with the hydraulic conductivity, pressure head, and soil water content, respectively. The linear variability is interpreted as an approximation of the linear component of real soil variability. Their scaling factors cause a linear transformation on each of the involved variables. It is assumed that the unexplained variability after this transformation was caused by the nonlinear component of the total variability. Eching et al. (1994) used the linear-variability concept in combination with the inverse technique to estimate *in situ* soil hydraulic properties in a 32-ha field. Measured

cumulative drainage curves were scaled yielding scaling factors. The hydraulic parameters of the reference profile were inversely estimated by numerically solving the scaled Richards' equation. Then the hydraulic parameters of the soil at another location can be determined using the scaling factors.

The similar-media concept introduced by Miller and Miller (1956) was derived from the theory of similarity. Similar media differ only in the scale of their internal geometry and have identical porosities. Warrick et al. (1977) extended the use of similar soils to soils with different internal geometries. Using the degree of saturation instead of volumetric moisture content eliminated the assumption of identical porosity. Simmons et al. (1979) based their work on the similarity between soil hydraulic functions instead of the similarity between respective internal geometries. Vogel et al. (1991) introduced a linear-variability concept and generalized the scaling relationships to enable their incorporation in numerical modeling of water movement in systems of parallel stratified one-, two-, or three-dimensional soil profile. Application of the transformation of Vogel et al. (1991) can capture the linear component of soil variability. For example, in the van Genuchten (1980) hydraulic relationship, the nonlinear component is characterized by the parameter n and its variability, which are ignored by Vogel et al. (1991). When the above methods are used to scale the soil hydraulic properties, scaling errors will be introduced. The amount of the error is determined by the similarity of the soil hydraulic properties. Because of this error, the hydraulic function obtained by an inverse scaling may be different from the original one.

We extended the linear-scaling method of Vogel et al. (1991) by introducing a non-similar media (NSM) scaling method. The hydraulic parameters of all the soil materials, regardless of their similarity, are scaled to a reference material. The soil variability is described by the scaling factors. Application of NSM scaling will reduce the number of parameters to be estimated in inverse modeling. The combination of the NSM scaling and the inverse procedure will allow the hydraulic parameters of the reference material to be estimated. The parameter values of each soil material can then be obtained by applying the inverse scaling.

2.0 Mathematical Relations

2.1 Hydraulic Functions

Soil hydraulic properties can be described by many empirical models, i.e., Brooks and Corey (1964 {1966 in Reference section}) and van Genuchten (1980). The commonly used van Genuchten (1980) function is expressed as

$$\theta(\psi) = \begin{cases} \theta_r + (\theta_s - \theta_r)\left[1 + (\alpha\,|\,\psi\,|)^n\right]^{-m} & \text{if} \quad \psi < 0 \\ \theta_s & \text{if} \quad \psi \geq 0 \end{cases} \tag{1}$$

where

θ	=	the volumetric water content
θ_s and θ_r	=	the saturated and residual water content
ψ [L]	=	water pressure head
α [L^{-1}] and n	=	fitting parameters that are inversely proportional to the air entry pressure value and the width of pore-size distribution of the medium, respectively
m	=	a constant that is commonly approximated by m = 1-1/n (van Genuchten 1980).

Combining Eq. (1) with the Mualem (1976) model yields the hydraulic conductivity function as

$$K(S_e) = K_s S_e^{\,0.5}\left[1 - \left(1 - S_e^{\,1/m}\right)^m\right]^2, \quad 0 \leq S_e \leq 1 \tag{2a}$$

or

$$K(\psi) = \begin{cases} K_s \dfrac{\left\{1 - (\alpha\,|\,\psi\,|)^{n-1}\left[1 + (\alpha\,|\,\psi\,|)^n\right]^{-m}\right\}^2}{\left[1 + (\alpha\,|\,\psi\,|)^n\right]^{0.5m}} & \text{if} \quad \psi < 0 \\ K_s & \text{if} \quad \psi \geq 0 \end{cases} \tag{2b}$$

where $K(\psi)$ [LT^{-1}] is the unsaturated hydraulic conductivity functions, and K_s [LT^{-1}] is the saturated hydraulic conductivity.

2.2 The Non-Similar Media Scaling

Different from the similar-media scaling (Miller and Miller 1956), the NSM scaling does not require the media to be similar. A soil that has M layers is composed of N (N ≤ M) different types of materials, each of which is associated with a set of hydraulic parameters. For example, if the van Genuchten (1980) hydraulic functions are used, the hydraulic parameters are (K_{si}, α_i, n_i, θ_{si}, θ_{ri}) for i = 1 to N, where i denotes a soil material with different hydraulic properties. We artificially select a set of reference values, $(\tilde{K}_s, \tilde{\alpha}, \tilde{n}, \tilde{\theta}_s, \tilde{\theta}_r)$, which may be the values of one of the N materials or other values. The linear scaling factors associated with the N soil materials are defined as

$$\gamma_{\beta_i} = \frac{\beta_i}{\tilde{\beta}} \tag{3a}$$

where β is any one of the hydraulic parameters, and γ is the scaling factor associated with parameter β for soil material i = 1 to N. The logarithmic scaling factors may be defined as

$$\left(\gamma_{\beta_i}\right)_{Ln} = \frac{Ln(\beta_i)}{Ln(\tilde{\beta})} \tag{3b}$$

The total number of the scaling factors is the same as the number of soil parameters. Note that selecting a different reference soil will produce different values of scaling factors. However, the actual parameter values and flow properties will not change. A diagram of the NSM scaling for a three-layer soil is shown in Figure 2.1. Totally, there are 15 parameters associated with the three layers (Figure 2.1a). These parameters can be described by 15 scaling factors and one set of reference parameter values (Figure 2.1b). As will be shown later, the scaling factors reflect the effects of soil layering, and the reference parameter values reflect the effects of spatial scale.

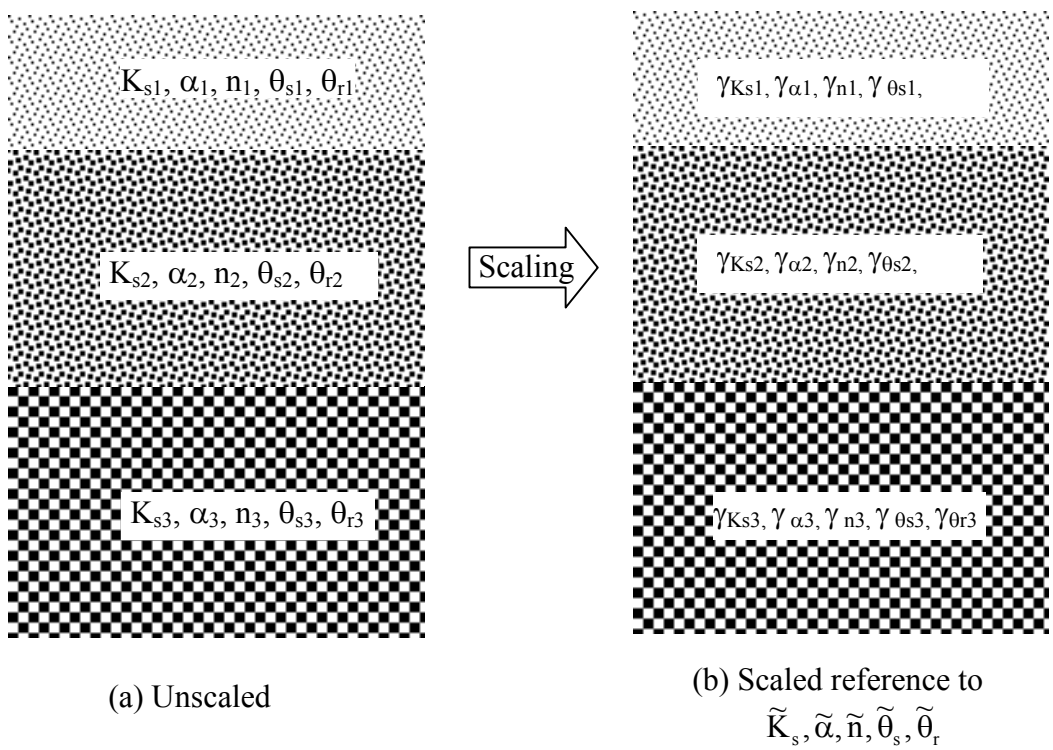


Figure 2.1. A Diagram that Shows NSM Scaling in Three-Layer Soil: (a) van Genuchten (1980) Parameters Before Scaling and (b) Scaling Factors and Reference Set of Parameters After Scaling

The NSM scaling has the following characteristics:

- NSM scaling does not require the constitutional materials to be similar. As long as the hydraulic properties of the soil materials can be described by a hydraulic function (e.g., Brooks and Corey 1964 {1966 in Reference section}; van Genuchten 1980), the NSM scaling is applicable.
- Instead of scaling the hydraulic properties (i.e., the $\theta(\psi)$ and $K(\psi)$) relations, the hydraulic parameters (e.g., parameters K_s, α, n, θ_s, and θ_r for the van Genuchten model) are scaled. As a result, the flow can always be expressed in real time and distance regardless of the soil heterogeneity. This overcomes the difficulty in estimating hydraulic parameters using an inverse procedure by minimizing the differences between the observed and predicted values.
- After the scaling, the values of the hydraulic parameters of all the soil materials perfectly reduce to the reference values. No scaling error is introduced, and hence the application of an inverse scaling will return the original parameter values.
- The spatial variability of each hydraulic parameter can be expressed by the scaling factors. Different parameters may have different variability structures.

2.3 Scaling Factors and the Observation Scale

The NSM scaling (Eq. 3) may be applied to the hydraulic parameters at different observation scales. By applying the NSM scaling to the local and field observation scales, we obtain

$$(\gamma_\beta)_{LS} = \frac{\beta_{Ls}}{\tilde{\beta}_{Ls}} \tag{4a}$$

and

$$(\gamma_\beta)_{FS} = \frac{\beta_{FS}}{\tilde{\beta}_{FS}} \tag{4b}$$

where β is any one of the hydraulic parameters, and the subscripts LS and FS denote for local-scale and field-scale, respectively. We assume that the values of the scaling factors at the local scale are approximately equal to those at the field-scale:

$$(\gamma_\beta)_{LS} \approx (\gamma_\beta)_{FS} \tag{5}$$

This means that the relative value of a parameter is constant at different observation scales. For example, if the local-scale K_s value of a soil material is larger than the value of the reference material, we expect that the field-scale value of K_s is also proportionally larger than the field-scale value of the reference material. Yeh et al. (1985) derived the effective hydraulic conductivity in a three-dimensional (3-D) steady-state infiltration in statistically isotropic unsaturated porous media. They showed that the effective hydraulic conductivity is linearly proportional to the mean value of the local-scale hydraulic conductivity for a given soil variability and correlation length (Eq. 43, Yeh et al. 1985). This suggests that Eq. (5) is true if the spatial variability and correlation length are the same for all the soil constitutional materials. Using Eq. (5), we can relate the values of the hydraulic parameters at different scales. This allows us to determine the scaling factors at an easily manageable scale (e.g., sample- or local-scale) using Eq. (4a)

and apply them to a case of a different observation scale (e.g., field scale). Note that the mean values of the local-scale parameters should be used to determine the scaling factors to minimize the measurement error. With the known scaling factors, the reference parameter values at the field scale, $\tilde{\beta}_{FS}$, can be estimated by inverse modeling. After this, the actual hydraulic parameter values at field-scale can be calculated by substituting the corresponding scaling factors and the reference values into Eq. (4b).

The specific method for determining the scaling factors for the experiments of Rockhold et al. (1988) and Abbaspour et al. (2000) using local observations will be described in detail in the Materials and Methods section.

2.4 Hydraulic Functions of Layered Soil

The hydraulic properties of each soil material can be described by Eqs. (1) and (2b). After applying the linear NSM scaling (Eq. 3a), the van Genuchten hydraulic functions for the heterogeneous soil is written as

$$\theta(\psi, z) = \begin{cases} \gamma_{\theta r}\tilde{\theta}_r + (\gamma_{\theta s}\tilde{\theta}_s - \gamma_{\theta r}\tilde{\theta}_r)\left[1 + (\gamma_\alpha \tilde{\alpha} \mid \psi \mid)^{\gamma_n \tilde{n}}\right]^{(1/\gamma_n \tilde{n} - 1)} & \text{if} \quad \psi < 0 \\ \gamma_{\theta s}\tilde{\theta}_s & \text{if} \quad \psi \geq 0 \end{cases} \tag{6}$$

and

$$K(\psi, z) = \begin{cases} \dfrac{\gamma_{Ks}\tilde{K}_s \left\{1 - (\gamma_\alpha \tilde{\alpha} \mid \psi \mid)^{\gamma_n \tilde{n} - 1}\left[1 + (\gamma_\alpha \tilde{\alpha} \mid \psi \mid)^{\gamma_n \tilde{n}}\right]^{(1/\gamma_n \tilde{n} - 1)}\right\}^2}{\left[1 + (\gamma_\alpha \tilde{\alpha} \mid \psi \mid)^{\gamma_n \tilde{n}}\right]^{0.5(1 - 1/\gamma_n \tilde{n})}} & \text{if} \quad \psi < 0 \\ \gamma_{Ks}\tilde{K}_s & \text{if} \quad \psi \geq 0 \end{cases} \tag{7}$$

where z is the soil depth. Note that the scaling factors are functions of soil depth, and the reference parameters take the values at corresponding field observation scale. We omit the argument z associated with γ_β and the subscript FS associated with $\tilde{\beta}_{FS}$ for the reason of brevity. Consequently, the θ-ψ and K-ψ are not one-to-one relationships any more for a layered soil. Using Eqs. (6) and (7), the 3-D Richards equation for a layered soil is written as

$$C(\psi, x, y, z)\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial x}\left[K_x(\psi, x, y, z)\frac{\partial \psi}{\partial x}\right] + \frac{\partial}{\partial y}\left[K_y(\psi, x, y, z)\frac{\partial \psi}{\partial y}\right] + \frac{\partial}{\partial z}\left[K_z(\psi, x, y, z)\frac{\partial \psi}{\partial z}\right] + \frac{\partial K_z(\psi, x, y, z)}{\partial z} \tag{8a}$$

where x and y are the horizontal coordinates, and z is the vertical coordinate positive downward; C is the water capacity defined as

$$C(\psi, x, y, z) = \frac{\partial \theta(\psi, x, y, z)}{\partial \psi} \tag{8b}$$

Note that all of the variables in Eq. 8a and 8b are expressed in dimensional forms. Thus, the model predictions and field observations are comparable. This enables the error between the predictions and the observations to be minimized, and hence the inverse modeling is applicable after the NSM scaling is applied.

2.5 Estimating the Field-Scale Reference Parameter Values

Nonlinear regression is needed when simulated values are nonlinear with respect to parameters to be estimated. The objective function is a measure of the fit between simulated values and is defined as

$$S(\beta) = \sum_{j=1}^{n_s} \sum_{i=1}^{n_j} w_{ij} [G_{ij} - \hat{G}_{ij}(\beta)]^2 \tag{9}$$

where

j	=	the different sets of measurements, that is, those involving water content or pressure head
n_j	=	the number of measurements in a particular set with n_s the number of measurement sets, which equals to 2 if the observations of θ and ψ are used
i	=	an observation
G_{ij}	=	ith measurement for the jth measurement set
$\hat{G}_{ij}(\beta)$	=	the corresponding model predictions
w_{ij}	=	the weights associated with measurement points and is defined as the reverse of the variance of the measurement error

The inverse problem is to minimize the objective function, $S(\beta)$, with respect to the soil hydraulic parameters.

For a layered soil, the number of the hydraulic parameters to be estimated using the inverse procedure can be reduced by applying the NSM scaling. The hydraulic functions for the whole soil domain are expressed in terms of the reference hydraulic parameters and the scaling factors associated with each of the component materials (Eqs. 6 and 7). Then the differential equation (Eq. 8) using these hydraulic functions will be solved during the inverse flow modeling. The objective function (Eq. 9) is minimized to estimate the values of the reference hydraulic parameters, $\tilde{\beta}_{FS}$.

3.0 Methods

3.1 STOMP/UCODE

The inverse modeling program UCODE (Poeter and Hill 1998) was developed by the U.S. Geological Survey in collaboration with the U.S. Army Corps of Engineers Waterways Experiment Station and the International Ground Water Modeling Center of the Colorado School of Mines. Any application model or set of models can be used. Application models can include preprocessors and postprocessors as well as models related to the processes of interest. A powerful aspect of using nonlinear regression is the useful statistics, which can be generated by UCODE. The statistics presented can be used diagnostically to measure the amount of information provided by the data and to identify model error (bias), or to infer the uncertainty with which values are calculated. UCODE performs a different function by assigning different PHASE values. The function of each PHASE is described briefly in Table 3.1. The optimized parameter values and their statistics are calculated when PHASE = 3.

Table 3.1. The Phases of UCODE and their Functions (modified from Poeter and Hill 1998)

PHASE	Function
1	Forward modeling using the starting parameter values.
11	Produces data sets from which objective-function contour graphs can be produced.
2	Sensitivities at starting parameter values using forward difference.
22	Sensitivities and parameter variances, covariance, and correlations at starting parameter values using central difference.
3	Performs inverse procedure to optimize the parameters to be estimated.
33	Calculates the modified Beale's measure of model linearity.
44	Calculates predictions and their linear confidence and prediction intervals.
55	Calculates differences and their linear confidence and prediction intervals.

The numerical simulator STOMP (White and Oostrom 2000) has been designed to solve a variety of nonlinear, multiple-phase, flow-and-transport problems for unsaturated porous media. The revised version of STOMP allows the input of scaling factors and the reference parameter values to simulate water flow. It also allows the inclusion of a UCODE Control Card and an Observed Data Card in the STOMP input file. By running STOMP, the universal (fn.uni) and the extract (fn.ext) files required by UCODE are constructed. STOMP also produces a new file (fn.sto) that includes the simulated values corresponding to the observations.

The UCODE prepare file (fn.pre) and the function file (fn.fnc) were constructed manually. When the number of observations was large, e.g., for the Sisson & Lu experiment described in the Application 3, an auxiliary program was written to construct the Observed Data Card in the input file for STOMP.

We use UCODE together with STOMP to inversely estimate the hydraulic parameters.

3.2 Method of Recursive Inversion

The scaling factors determined based on the local-scale measurements have inherited observation and sampling errors. Consequently, the estimated field-scale parameter values are not accurate. Thus, further optimization of the scaling factors may be needed after the field-scale reference parameters have been inversely estimated. Since the number of scaling factors usually is large for a heterogeneous soil, their simultaneous estimation is difficult to converge. We divide them into N_g groups, and the scaling factors of the first group are estimated inversely by fixing the values of the rest parameters. Then the scaling factors in the second group will be estimated. After the scaling factors of the last group are estimated, the estimation goes to the first group again. This process will continue until the convergence criterion is satisfied. This process is called recursive inversion since multiple times of inversion are required.

4.0 Applications and Results

4.1 Application 1 - Homogeneous Soil

A drainage experiment was carried out in the North steel caisson (Rockhold et al. 1988) at the Buried Wastes Test Facility (BWTF). The caisson was 7-m long and 2.7-m in diameter. It was filled with a relatively uniform material, consisting of approximately 97% sand, 2% silt, and 1% clay. Neutron probe readings were taken every 30 cm until 240 cm plus one at 45 cm. Tensiometer readings were taken every 30 cm till 180 cm plus two at 15 and 45 cm.

The hydraulic properties of the same soil were also measured in the laboratory by packing the soil to prescribed bulk density in an acrylic cylinder of known volume. Soil water contents, pressure head, and water flux were measured at multiple times, of which the flow was under steady state. The parameter values from the lab experiments were determined by simultaneously fitting the $K(\psi)$ and $K(\theta)$ hydraulic functions using MathCad 8. The parameter values from the field experiment were estimated by inverse modeling using UCODE/STOMP.

The hydraulic functions of the BWTF soil at the lab-scale and the field-scale are shown in Figure 4.1. The differences of the hydraulic properties between the lab- and field-scale are that 1) the value of θ_s at lab-scale (0.438 m^3m^3) is significant larger than that at field scale (0.308 m^3m^3), 2) the air-entry pressure is not shown at the lab-scale ψ-θ curve but is shown at the field-scale ψ-θ curve, and 3) the values of parameter n at the field-scale are more than double those measured at the lab-scale. The differences of the rest three parameters are relatively small at the two observation scales.

Figure 4.2 compares the predicted and the observed water contents and pressure heads of the BWTF drainage experiment (Rockhold et al. 1988) using both the lab-scale and field-scale hydraulic parameter values. When the lab-scale parameter values were used, soil water contents were overestimated (Figure 4.2a) and most of the pressure heads were underestimated (Figure 4.2c). When the field-scale parameter values were used, both water contents (Figure 4.2b) and pressure head (Figure 4.2d) were well predicted.

4.2 Application 2 - Layered Soil

The Grass site of Rockhold et al. (1988) is located approximately 4 km southwest of the BWTF. The uppermost 0.6 m of the soil profile contains approximately 74% sand, 21% silt, and 5% clay, and is classified as sandy loam to loamy sand. From 0.6 to 3.5 m, the soil consists of approximately 91% sand, 6% silt, and 3% clay, and is classified as sand. The drainage experiment was conducted at a site of 2×2 m with a neutron probe access tube in the center. Tensiometers were placed at 0.15- to 0.30-m-depth increments, down to 1.8 m. Using planking installed in narrow trenches facilitated ponding, around which soil was thoroughly compacted. Water contents were monitored with a model 503DR Hydro-probe (Campbell Pacific Nuclear Corp., Martinez, California). Pressure heads were measured with tensiometers and a Tensimeter (Soil Measurement Systems, Tucson, Arizona) pressure transducer. Tensiometer and Neutron probe readings were taken every 10 to 15 min during the initial drainage phase of the experiment and less frequently as time passed (Rockhold et al. 1988). The water content and pressure-head data of their Tables A.7 and A.8, respectively, were used in our modeling. The pressure-head observations at 0.15 and 1.80 m were set as the upper and lower boundaries, respectively. Note that we intentionally did

not use the zero flux as the upper boundary because of the possible existence of other processes of water flow (e.g., transpiration) other than drainage (Rockhold et al. 1988).

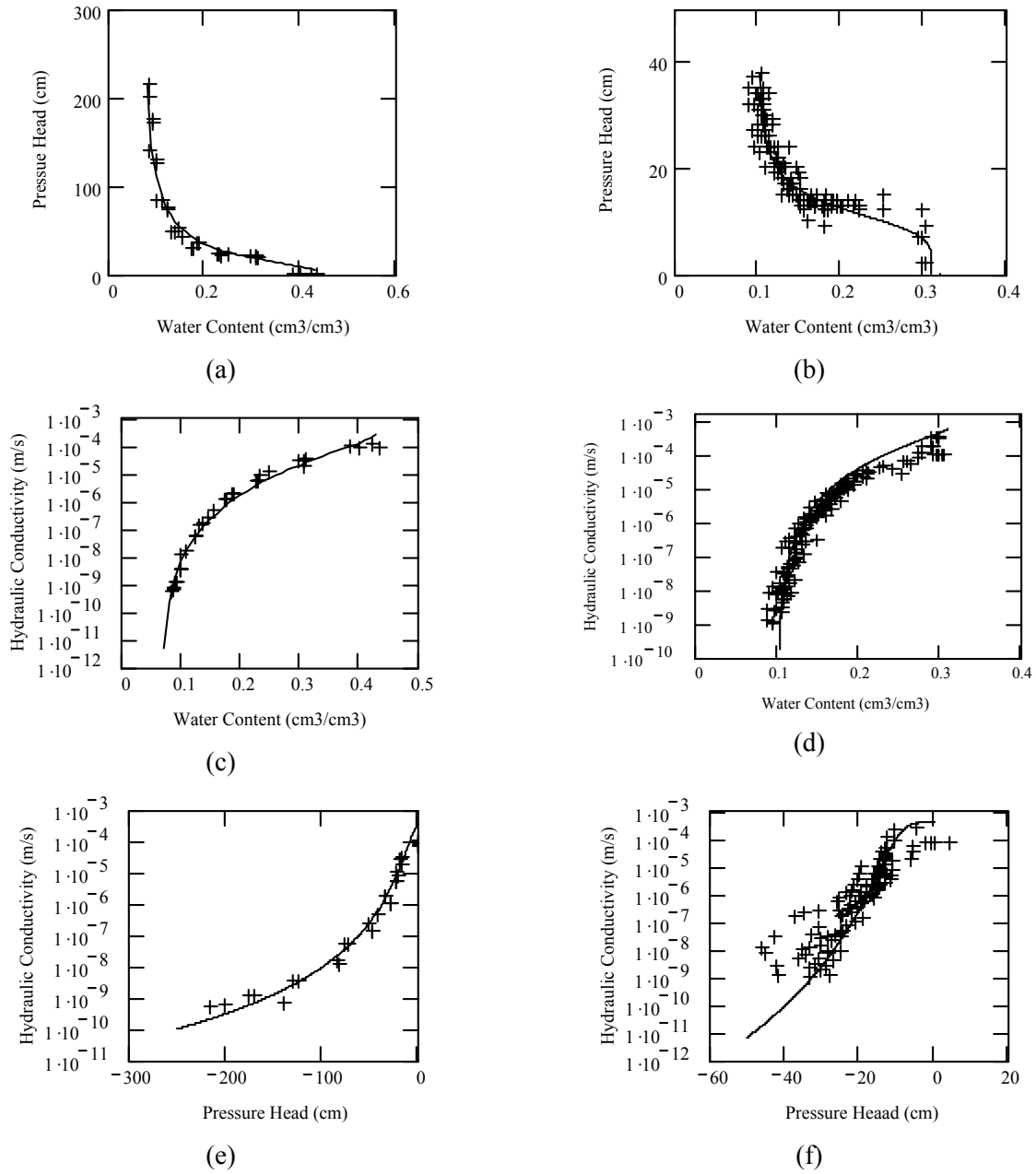


Figure 4.1. The Hydraulic Properties of the BWTF Soil at the Lab Scale (a, c, and e) and Field Scale (b, d, and f). Lab-scale parameter values: $K_s = 3.163\times10^{-4}$ ms^{-1}, $\alpha = 6.42$ m^{-1}, $n = 2.185$, $\theta_s = 0.438$ m^3m^{-3}, and $\theta_r = 0.063$ m^3m^{-3}. Field-scale parameter values: $K_s = 3.376\times10^{-4}$ ms^{-1}, $\alpha = 8.61$ m^{-1}, $n = 4.886$, $\theta_s = 0.308$ m^3m^{-3}, and $\theta_r = 0.101$ m^3m^{-3}.

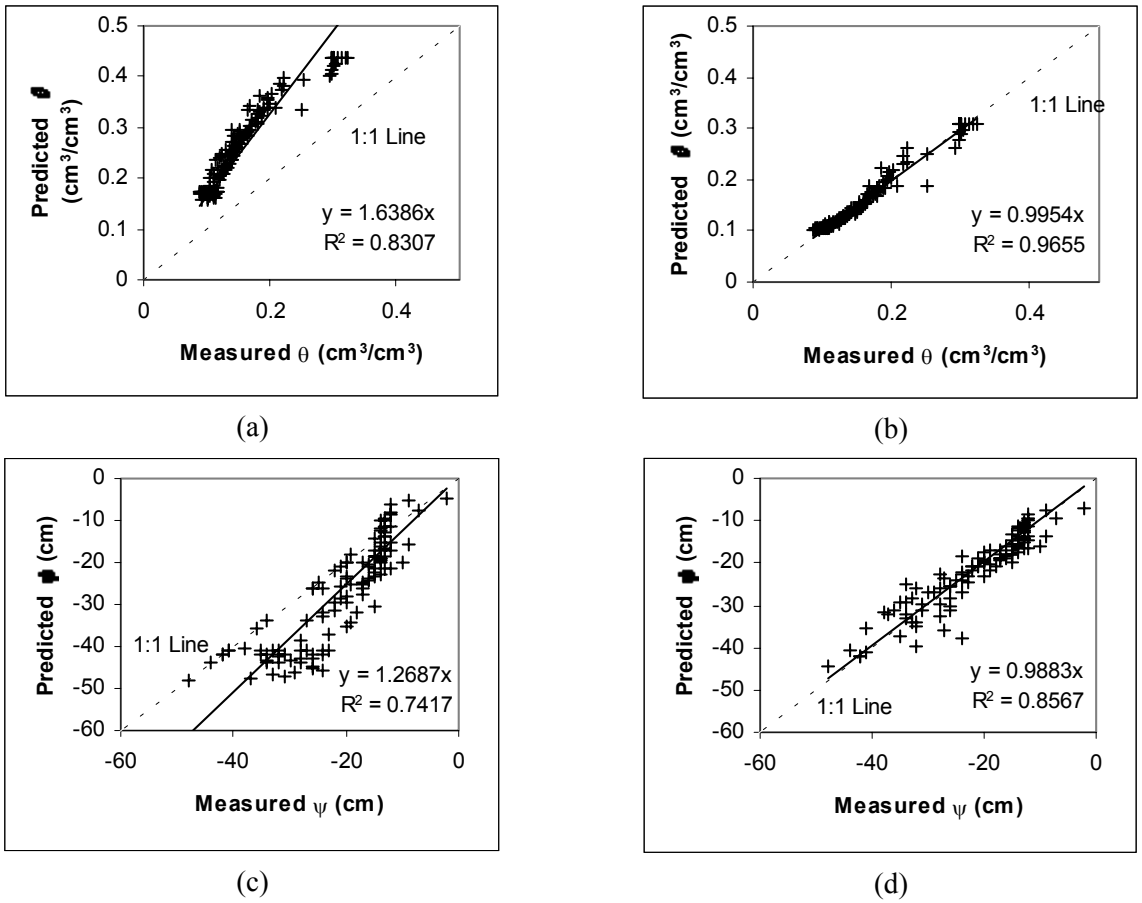


Figure 4.2. Comparisons of the Predicted and Field Measured Water Contents and Pressure Heads of the BWTF Drainage Experiment (Rockhold et al. 1988) Using the Lab-Scale Hydraulic Parameter Values (a and c) and the Field-Scale Hydraulic Parameter Values (b and d). Dashed lines: the 1:1 line. Solid lines: linear-regression line.

The local-scale parameter values of α, n, θ_s, and θ_r at each soil depth (Table 4.1) were obtained by fitting the soil-water retention curves using MathCAD® 8. We arbitrarily selected the parameter values of the top layer as the reference to calculate the scaling factors of the four parameters using Eq. (2b). Then the scaling factors of K_s were determined using the best fits of these four parameters of each layer and the steady-state observations of θ and ψ. The steady state occurred at the beginning of the drainage process. At steady state, the water flux passing through each layer was the same and equals to the unsaturated hydraulic conductivity at the corresponding layer:

$$q_0 = K(\psi) \tag{10}$$

where q_0 is the steady-state flux, which may not be known. The use of the van Genuchten (1980) hydraulic function and Eq. (10) yields

$$K_{s\theta} = q_0 \cdot S_{e0}^{-0.5}\left[1-\left(1-S_{e0}^{1/m}\right)^m\right]^{-2}, \quad 0 \le S_e \le 1 \tag{11a}$$

and

$$K_{s\psi} = \begin{cases} q_0 \cdot \dfrac{\left[1+(\alpha\,|\,\psi_0\,|)^n\right]^{0.5m}}{\left\{1-(\alpha\,|\,\psi_0\,|)^{n-1}\left[1+(\alpha\,|\,\psi_0\,|)^n\right]^{-m}\right\}^2} & \text{if} \quad \psi < 0 \\ q_0 & \text{if} \quad \psi \ge 0 \end{cases} \tag{11b}$$

where the subscript zero denotes the observation at steady state with flux of q_0, and $K_{s\theta}$ and $K_{s\psi}$ are the estimated values of K_s using the observations of θ and ψ, respectively. Note that $K_{s\theta}$ and $K_{s\psi}$ may not be the same because of the experiment error. The scaling factors of K_s were calculated by

$$\gamma_{Ks_i} = \frac{N \cdot K_{si}}{\sum_{i=1}^{N} K_{si}}. \tag{12}$$

where the subscript i denotes different soil layers. Note that the variable q_0 will be cancelled in Eq.(12). Applying Eqs. (11a) and (11b) to (12) will produce two sets of scaling factors associated with K_s of each soil layer. We used the average of the corresponding values of the two sets of scaling factors in our modeling.

Table 4.1. The Values of the Hydraulic Parameters at Local Scale and Calculated Scaling Factors Reference to the First Layer of the Soil at the Grass Site (Rockhold et al. 1988)

		Layer 1	**Layer 2**	**Layer 3**	**Layer 4**
Parameter Values	K_s (ms^{-1})	1×10^{-5}	4.29×10^{-7}	2.56×10^{-7}	1.05×10^{-7}
	α (m^{-1})	8.41	7.85	12.72	13.13
	n (-)	1.232	1.236	1.355	2.054
	θ_s (m^3m^{-3})	0.264	0.199	0.153	0.146
	θ_r (m^3m^{-3})	0.043	0.022	0.017	0.031
	S_r^+ (-)	0.163	0.111	0.111	0.212
Scaling Factors	γ_{Ks}	1	0.0429	0.0256	0.0105
	γ_α	1	0.933	1.512	1.561
	γ_n	1	1.003	1.100	1.667
	$\gamma_{\theta s}$	1	0.754	0.580	0.553
	γ_{Sr}	1	0.681	0.681	1.301

For comparison, the K_s value at the local scale for the top layer of the grass site soil was approximated by the measurement of the Guelph Permeameter method conducted within this layer (Rockhold et al. 1998 {1988 in Reference list and in other callouts}).

Controlled by the inverse model UCODE, the Richards equation is solved numerically using STOMP and parameter estimates are sought by minimizing the differences between the predictions and the observations. Using the values of the scaling factors in Table 4.1, the best estimates of the reference hydraulic parameters at field scale and their corresponding 95% linear confidence interval (LCI) are given in Table 4.2. The range of the 95% LCI shows the precision of the estimates. A larger range of 95% LCI means less precise estimation of the parameter. Note that parameters $\tilde{K}_s$, $\tilde{\alpha}$, and $\tilde{n}$ were log-transformed, and hence their 95% LCIs are expressed as the mean values multiplied or divided (×/÷) by a factor, which has the minimum value of unity. In Table 4.2, the 95% LCI for parameter $\tilde{K}_s$ has the largest uncertainty, which varies with a factor of 1.57. The 95% LCI for the parameter $\tilde{\alpha}$ varies with a factor less than 1.18. Parameters $\tilde{n}$, $\tilde{\theta}_s$, and $\tilde{S}_r$ have relatively small ranges of 95% LCI. Note that the 95% LCI may be different from the actual 95% confidence interval (CI) since the water flows are nonlinearly related to hydraulic parameters.

Table 4.2. The Inversely Determined Field-Scale Reference Values of the Hydraulic Parameters with 95% LCI, the Ratios of the Reference Parameter Values at the Field Scale to those at Local Scale, and the Composite Scaled Sensitivities (CSS) of Each Parameter

Parameters	Mean with 95% LCI	$\tilde{\beta}_{FC} / \tilde{\beta}_{LC}$	CSS
$\tilde{K}_s$	2.787×/÷1.57 (10^{-3} ms^{-1})	279	8.25
$\tilde{\alpha}$	11.27×/÷1.18 (m^{-1})	1.34	9.19
$\tilde{n}$	1.214×/÷1.04	0.99	8.23
$\tilde{\theta}_s$	0.258±0.011 (m^3m^{-3})	0.98	2.30
$\tilde{S}_r$	0.213±0.039	1.31	1.35
$\tilde{\theta}_r$	0.055† (m^3m^{-3})	1.31	–
† $\theta_r = S_r\theta_s$			

The reference parameter values in Table 4.2 can also be thought to be the optimized parameter values of the top layer at the experiment scale. The field-scale value of the K_s is 279 times of the local scale value measured using the Guelph Permeameter method. There are two possible reasons for the large difference. One is that local-scale value of K_s was not well determined. The other is that the scale effect is quite large for K_s. The field-scale values of $\tilde{\alpha}$ and $\tilde{S}_r$ are 34% and 31% larger than the corresponding local-scale values, respectively. Parameters $\tilde{n}$ and $\tilde{\theta}_s$ have almost identical values at the two observation scales. This suggests that the values of the hydraulic parameters at field scale may be very

different from the values at local scale. The hydraulic parameters have a scale effect because of the existence of soil heterogeneity and the nonlinear effects of the heterogeneity on water flow. Although the soil profiles were divided into a few soil layers, mild heterogeneity still exists within a layer. If the soil layers were perfectly homogeneous, there would not be any scale effect.

Using the values of the scaling factors in Table 4.1 and the field-scale reference parameters in Table 4.2, the values of the hydraulic parameters for each soil layer at the experimental scale were calculated. These values can be used to predict the field-scale soil-water retention curves of each soil layer. Figure 4.3 shows the comparison between the observed local-scale and predicted field-scale water-retention curves. The curvature of the field-scale curve for Layer 1 is slightly different from the trend of the local-scale curve. The local-scale and field-scale curves for the rest layers are very similar. Generally, the main characteristics of the water-retention curves are similar at the local scale and at the field scale.

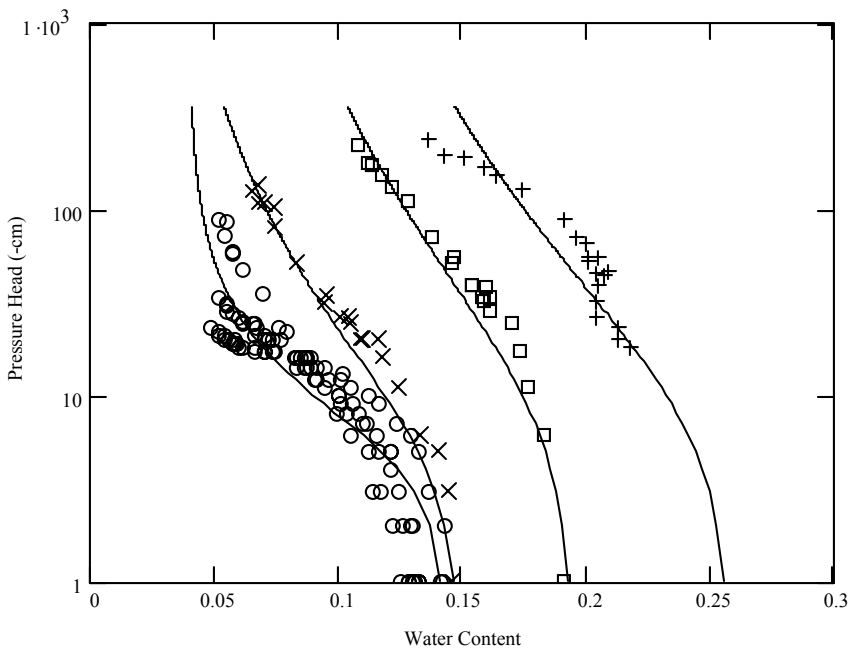


Figure 4.3. The Measured and Predicted Soil-Water Retention Curves of each Layer at the Grass Site of Rockhold et al. (1988)

One problem of using the inverse procedure is the probable non-uniqueness of the estimates of the parameters, which is due to the high correlation between some of the parameters. Correlation coefficients (R) range in value from –1.0 to 1.0. The values of R close to -1.0 or 1.0 indicate that the parameter values cannot be uniquely estimated with the observations used in the regression. The maximum correlation coefficient (R = 0.93) between the reference hydraulic parameters occurred between $\tilde{K}_s$ and $\tilde{\alpha}$. The absolute values of the rest correlation coefficients are equal or less than 0.70. According to Hill (1998), the value of R less than 0.95 suggests that non-uniqueness is not a problem. Thus, the estimates of the field-scale reference parameters are likely to be unique.

4.2.1Predictions of Flow

Although the soil-water retention curves for each soil layer are similar at the local and field scales, the prediction of flow is very different, mainly due to the large difference of the K_s values at the local- and field-scale. Comparisons between the observations and the predictions are shown in Figure 4.4. Perfect correlation between the predictions and the observations has the intercept of zero, the slope of unity, and the correlation coefficient of unity. When the local-scale parameter values are used, both soil-water contents and pressure head were significantly overestimated. When the field-scale parameter estimates obtained by the inverse method were used to predict the flow, the prediction errors were much smaller than those using the local-scale parameter values. Comparisons between the observations and the predictions calculated using the field-scale parameter values are shown in Figure 4.4b and Figure 4.4d. The slopes of the trend lines are 0.956 to 0.997 for θ and ψ, respectively. This indicates that the systematic bias of prediction using the local-scale parameter values has been removed.

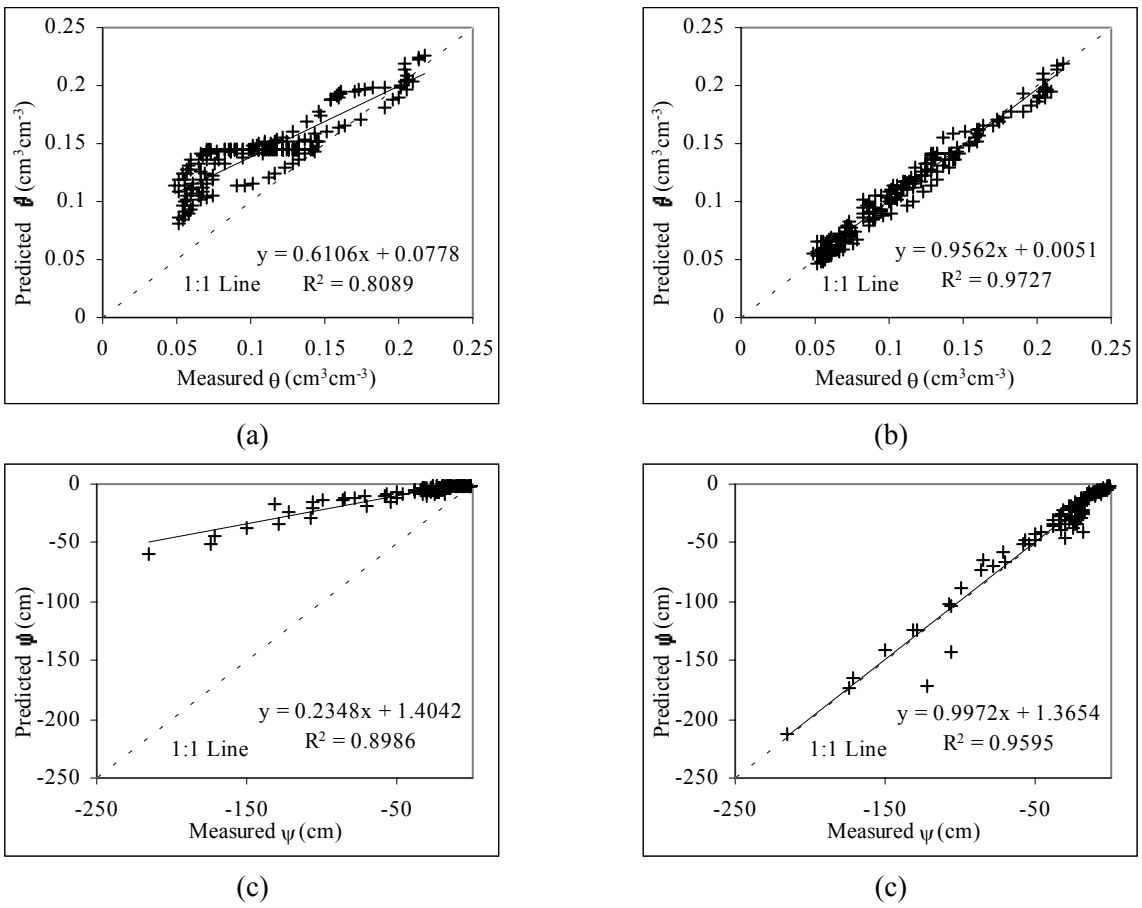
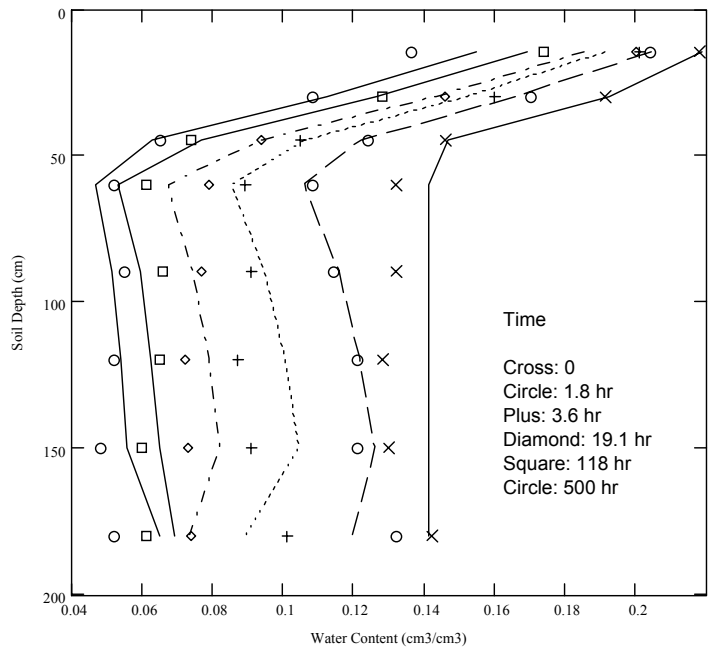
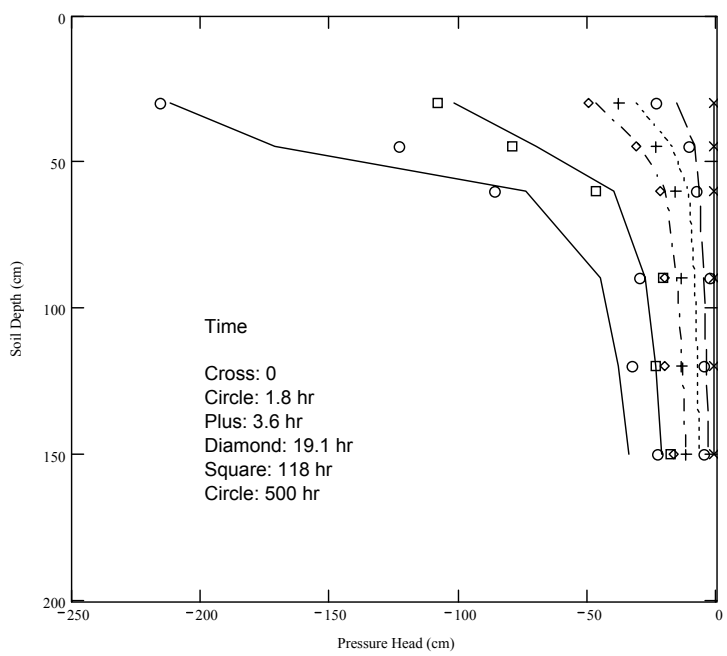


Figure 4.4. Comparisons of the Predicted and Field Measured Water Contents and Pressure Heads of the Grass Site Drainage Experiment (Rockhold et al. 1988) Using the Lab-Scale Hydraulic Parameter Values (a and c) and the Field-Scale Hydraulic Parameter Values (b and d). Dashed lines: the 1:1 line. Solid lines: linear regression line.

To examine the spatial and temporal distribution of prediction error when the field-scale parameter values were used, the observations and predictions of flow at different time and soil depth are plotted in Figure 4.5. Generally, there is no clear temporal effect on the prediction error. However, minor spatial effects exist. The water contents at the soil below 60 cm have a relatively larger prediction error than those above 60 cm (Figure 4.5a). The reason is that the soil below 60 cm was treated as one layer while that above was treated as three layers with different properties. The heterogeneity that existed in the soil below 60 cm may be slightly larger than that in the rest layers. However, this small heterogeneity does not affect the predictions of pressure head in this layer by much (Figure 4.5b).



(a)



(b)

Figure 4.5. Comparison of the Observed and the Predicted Values of (a) Water Content and (b) Pressure Head of the Drainage Experiment Conducted at the Grass Site by Rockhold et al. (1988)

4.3 Application 3 - Heterogeneous Soil

In 1980, an injection experiment was conducted at the Hanford 200 East Area. The experiment was described in Sisson and Lu (1984). A solution containing multiple tracers was injected at a single point into the subsurface sediments. The resulting spread of the water and tracers was monitored in 32 wells that surrounded the injection point, which was at the depth of 4.57 m (15 ft) below the ground surface. The monitoring wells extended from the surface to a depth of 18.3 m (60 ft). Eleven injection tests were performed. The injection rates ranged from 270 to 420 L/h (2.5 to 3.9 gal/h). The water content was measured with neutron probes, and the concentrations of the radioactive tracers were measured with a gamma energy analysis probe. Measurement depths of water contents ranged from 0.3 to 18.3 m (1 to 60 ft) at the interval of 0.3048 m (1 ft).

The proposed non-similar scaling method and the inverse procedure using UCODE/STOMP are tested by modeling the water flow of a small section of the Sisson and Lu site. This section includes four observation wells marked by H2, H4, H6, and H8, respectively. The lab-scale parameter values were measured using the cores described in Last and Caldwell (2001). The soil zonation was taken according to the K_s values of these cores. The soil materials are classified into five texture groups, whose lab-scale hydraulic parameter values and their occurrence depths are listed as Case I in Table 4.3. A 2-D cylindrical coordinate system was used with the origin at the depth of 15.24 m (50 ft) directly below the injection well. Non-uniform cell sizes are assigned and varied from 0.1 m to 0.5 m at the radial (r) direction and from 0.1524 m (0.5 ft) to 0.3048 m (1 ft) at the vertical direction (z). The 519 observations from the first two injections were used to inversely estimate the field-scale soil hydraulic parameters. The observations about 3 months before the start of the experiment were taken as the initial values. A zero-flux top boundary and a unit-gradient lower boundary were assigned to the surface of the soil and at the depth of 15.24 m (50 ft), respectively. Five constitutional soil materials (Table 4.3) with different textures were assigned to the region to be simulated. We assume that 1) the soil layers are horizontal, 2) the soil materials are anisotropic, and each of them has a unique set of hydraulic parameters, 3) the scaling factors associated with K_{sh} and K_{sv} are the same, where K_{sh} and K_{sv} are the horizontal and vertical saturated hydraulic conductivity, respectively, and 4) the source strength to the H section is equal to the average source strength.

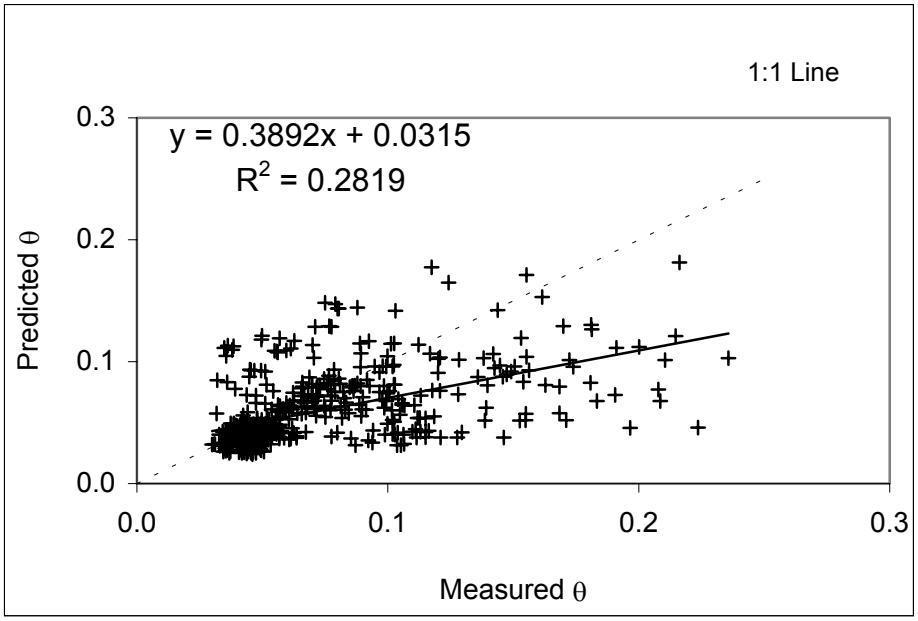
Three parameterization cases were considered. The field-scale parameter values were 1) equal to the lab-scale parameter values, 2) obtained inversely by applying the NSM scaling, and 3) obtained by applying the NSM scaling and recursive inversion. The parameter values for the three cases are listed in Table 4.3. Comparisons of the predicted and observed soil-water contents for the cases are shown in Figure 4.6. When the lab-scale parameter values were used to predict the flow (Figure 4.6a), there is a very low correlation between the predictions and observations ($R^2 = 0.28$). When the field-scale parameter values were obtained by applying the NSM scaling, the correlation between the predictions and observations ($R^2 = 0.45$) was improved (Figure 4.6b). After applying the NSM scaling taking the

recursive inversion, the accuracy of the field-scale parameter values was significantly improved (Figure 4.6c). This is shown by the high correlation between the predictions and observations ($R^2 = 0.74$, Figure 4.6c). The standard deviation was 0.0175 m^3m^{-3}, and the 95% linear confidence interval (LCI) was ± 0.034 m^3m^{-3}. However, some problems exist. On average, the soil-water content was underestimated. This suggests that the actual source strength at the H-section is larger than the average source strength assigned in the simulation. The water contents in material B were predicted poorly ($R^2 = 0.39$, not shown). The possible reason is that the distribution of this material was not assigned correctly. The predictions get poorer as the horizontal distance to the injection well becomes larger. This may be because of the assumption that the soil layers were horizontal while the actual thickness of a soil layer varies three-dimensionally. Therefore, for more accurate simulation, a 3-D model should be used. The soil texture distribution should reflect the 3-D soil heterogeneity; for example, according to the data from seismic imaging that provide detailed information on the lithology and structure.

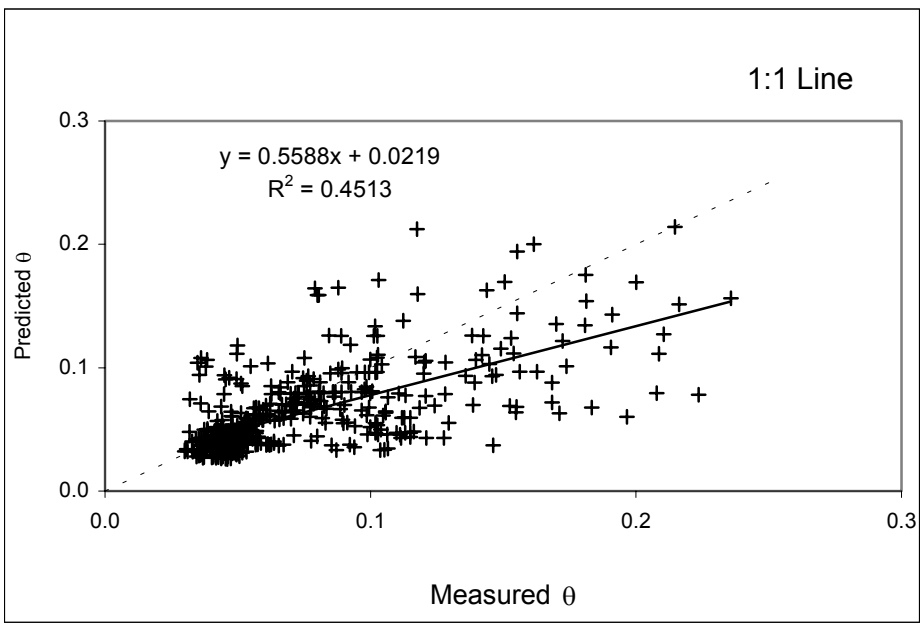
Table 4.3. The Soil Materials and the Corresponding Hydraulic Parameter Values of the H-Section of the Sisson & Lu Site (Sisson and Lu 1984). Parameters θ_s and θ_r were kept the same as the lab-scale values for all the three cases. Parameterizations: (I) lab-scale parameter values; (II) field-scale parameter values obtained inversely by applying the NSM scaling; and (III) field-scale parameter values after the recursive inversion.

		Material Number				
		B	**C**	**D**	**E**	**F**
	Soil Depth (ft)	18.0-19.5, 22.0-23.0, 31.0-32.0, 32.5-33.0, 36.0-38.5	0.0-12.0, 19.5-20.0, 29.0-30.0, 32.0-32.5, 33.0-33.5, 34.5-36.0	12.0-18.0, 20.0-20.5, 21.0-22.0, 23.0-25.5, 33.5-34.5	20.5-21.0, 26.0-29.0, 30.0-31.0, 38.5-39.0, 40.0-50.0	25.5-26.0, 39.0-40.0
	θ_s(m^3m^{-3})	0.338	0.364	0.368	0.373	0.41
	θ_r(m^3m^{-3})	0.036	0.035	0.033	0.027	0.02
Case I	K_s (ms^{-1})	1.78×10^{-5}	5.05×10^{-5}	1.99×10^{-4}	4.90×10^{-4}	1.05×10^{-3}
	α (m^{-1})	4.7	8.6	8.9	6.9	20.0
	n (-)	2.063	1.995	2.958	3.739	3.05
Case II	K_{sh} (ms^{-1})	4.01×10^{-5}	1.14×10^{-4}	4.48×10^{-5}	1.10×10^{-3}	2.37×10^{-3}
	K_{sv} (ms^{-1})	1.46×10^{-5}	4.14×10^{-5}	1.63×10^{-4}	4.01×10^{-4}	8.60×10^{-4}
	$\alpha^{\dagger}$ (m^{-1})	4.7	8.6	8.9	6.9	20.0
	n (-)	1.934	1.870	2.773	3.504	2.859
Case III	K_{sh} (ms^{-1})	1.23×10^{-3}	1.34×10^{-5}	1.64×10^{-3}	1.38×10^{-4}	7.09×10^{-4}
	K_{sv} (ms^{-1})	4.44×10^{-4}	4.84×10^{-6}	5.92×10^{-4}	4.99×10^{-5}	2.56×10^{-4}
	α (m^{-1})	33.4	2.6	7.5	3.5	9.4
	n (-)	1.621	3.95	2.956	3.144	2.134

† α was fixed due to the high correlation between α and K_{sh}.

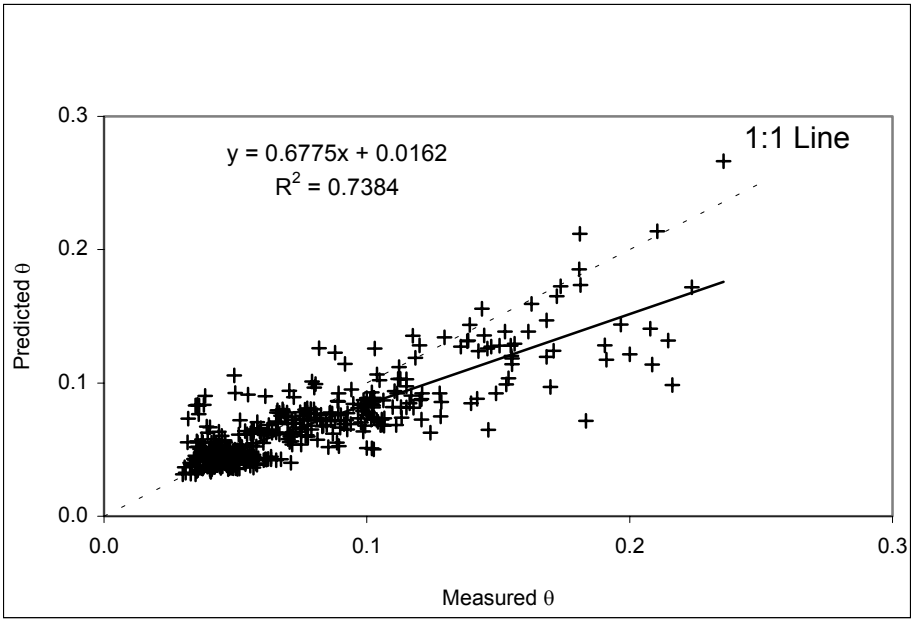


(a)



(b)

Figure 4.6. Comparison of the Predicted and Observed Soil Water Contents at the H-Section of the Injection Experiment Described in Sisson and Lu (1984). Parameter values for each case are listed in Table 4.3. The number of observations N = 519. Parameterizations: (I) lab-scale parameter values; (II) field-scale parameter values obtained inversely by applying the NSM scaling; and (III) field-scale parameter values after the recursive inversion. Dashed lines: the 1:1 line. Solid lines: linear regression line.



(c)

Figure 4.6 (Contd)

5.0 Summary and Conclusions

The accurate prediction of water flow and contaminant transport in unsaturated porous media is hampered by insufficient and uncertain constitutive property information. We proposed an NSM scaling method that can be coupled with inverse-flow modeling to estimate constitutive parameters for heterogeneous soils. By assigning the scaling factors to the same soil layers in the field, the reference hydraulic-parameter values at field scale can be estimated through inverse modeling of well-designed field experiments. Parameters for individual layers are then obtained through inverse scaling of the reference values using the *a priori* relationships between the reference parameter values and the specific value for each layer.

The numerical simulator, STOMP, was combined with the inverse modeling program, UCODE, to estimate the hydraulic parameters. Three cases of soil heterogeneity, i.e., homogeneous soil, layered soil, and heterogeneous soil, were considered. For the drainage experiment in the North Caisson with homogeneous soil near BWTF, soil-water contents (θ) were overestimated, and most of the pressure heads (ψ) were underestimated when the lab-scale parameter values were used. When the field-scale parameter values were used, both θ and ψ were well predicted. For the drainage experiment in the Grass Site with layered soil, both soil water contents and pressure head were significantly overestimated when the local-scale parameter values are used. When the field-scale parameter estimates obtained by the inverse method were used to predict the flow, the prediction errors were much smaller than those using the local-scale parameter values. The slopes of the trend lines between the observed and predicted values were 0.956 to 0.997 for θ and ψ, respectively. Preliminary work has been conducted to estimate the hydraulic parameters of a small section of the Sisson and Lu site in the 200East area. When the lab-scale parameter values were used to predict water contents, there was a very low correlation between the predictions and observations ($R^2 = 0.28$). This correlation was significantly improved ($R^2 = 0.74$) when the inversely estimated field-scale parameter values were used. The standard deviation was 0.0175 m^3m^{-3}, and the 95% LCI was ± 0.034 m^3m^{-3}. For a more accurate simulation, a 3-D model should be used. The soil-texture distribution should reflect the 3-D soil heterogeneity, for example, according to the data from seismic imaging that provide detailed information on the lithology and structure.

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