Stochastic Hydrology and Hydraulics 12 (1998) 285–298 © Springer-Verlag 1998

A geostatistically based inverse model for three-dimensional variably saturated flow

Debra L. Hughson, T.-C. Jim Yeh

Abstract We present a geostatistically based inverse model for characterizing heterogeneity in parameters of unsaturated hydraulic conductivity for three-dimensional flow. Pressure and moisture content are related to perturbations in hydraulic parameters through cross-covariances, which are calculated to first-order. Sensitivities needed for covariance calculations are derived using the adjoint state sensitivity method. Approximations of the conditional mean parameter fields are then obtained from the cokriging estimator. Correlation between parameters and pressure – moisture content perturbations is seen to be strongly dependent on mean pressure or moisture content. High correlation between parameters and pressure data was obtained under saturated or near saturated flow conditions, providing accurate estimation of saturated hydraulic conductivity, while moisture content measurements provided accurate estimation of the pore size distribution parameter under unsaturated flow conditions.

1 Introduction

Difficulty in detailed characterization of spatially varying hydraulic properties of field sites remains one of the main challenges for successful prediction of flow and transport in the vadose zone. Characterizing the vadose zone in detail using core samples or small-scale hydraulic tests is prohibitively time-consuming and costly and, consequently, is beyond the means of most studies. For these reasons there has been much interest and research into using the more easily measured states of the flow system, i.e. pressure head and moisture content, to estimate soil hydraulic properties. In the following discussion we refer to the soil hydraulic properties as primary information and measured states of the flow system as secondary information. This use of secondary information for the purpose of determining hydraulic properties of the porous medium is the essence of the so-called 'inverse problem' in subsurface hydrology. While the field scale inverse problem is inherently ill-posed and the solution non-unique, the difficulties en-

D.L. Hughson, T.-C. Jim Yeh
Department of Hydrology and Water Resources,
The University of Arizona

Correspondence to: D.L. Huglison
Funding for this research was provided by U.S. Department of Energy Environmental Science Management Program (ER-EM-EMSP-96) under contract AV-0655 with Sandia National Laboratories. The authors are grateful to Mauro Giudici for his thorough review of the manuscript and insightful and constructive comments.

countered in inverse modeling of flow in the vadose zone are exacerbated due to the nonlinearity introduced by the pressure-hydraulic conductivity relationship for unsaturated flow.

Recently some success in estimating hydraulic properties using data of moisture content and water pressure has been attained by means of the geostatistical approach to the inverse problem (e.g., Yeh and Zhang, 1996). The advantage of the geostatistical approach is that its solution to the inverse problem is unique and approximates the conditional mean of the hydraulic property fields. The approach, however, is limited by the fact that cokriging is a linear estimator while the relationship between hydraulic properties and secondary information in unsaturated porous media is highly nonlinear. As a result, the usefulness of the secondary information is not fully exploited. To circumvent this problem, Zhang and Yeh (1997) developed an iterative technique, which incorporates the nonlinearity into the cokriged estimate, such that more detailed and accurate hydraulic property fields can be produced than with the linear estimator from the same secondary information. However, for small parameter variance iteration does not result in much improvement since the relationship between primary and secondary information in this case is nearly linear and is well-described by the cokriging estimator.

While these results appear promising, much work remains to be done. First, the Gardner model of unsaturated hydraulic conductivity used by Yeh and Zhang (1996) and Zhang and Yeh (1997) is convenient due to its mathematical simplicity but fails to accurately portray the pressure – hydraulic conductivity and water content behavior observed in many types of geological media. In addition, only two-dimensional steady flow regimes have been considered in previous studies but flow in the vadose zone is inherently three-dimensional and time-dependent. Therefore, the objective of this study is to extend the geostatistical inverse model of Yeh and Zhang (1996) for two-dimensional steady flow to three-dimensional transient flow regimes. We further include a more realistic model for the pressure-hydraulic conductivity and pressure-water content relationships (van Genuchten, 1980). This enhancement allows for more accurate modeling of soil water pressure – hydraulic conductivity behavior and, perhaps, more accountability for the effect of variability of soil properties. It should be noted that the new aspects of the model presented here are its three-dimensionality, time-dependence, and incorporation of the van Genuchten relative hydraulic conductivity function. Following the model development we present tests of its validity using one-dimensional fully determined inverse problems. Model utility is then demonstrated using three-dimensional steady state stochastic inverse problems for small variances of parameter heterogeneities.

2
Mathematical formulation

Flow of water in partially saturated porous media is described by

$$(\beta S_s + C(\psi))\frac{\partial\psi}{\partial t} = \nabla \cdot (K(\psi)\nabla(\psi + z)) \tag{1}$$

In this expression ψ is pressure head, which is positive when soil is fully saturated and is negative when the soil is partially saturated, and z is the vertical coordinate positive in the upward direction. The term S_s represents specific storage and β is one when ψ is positive and zero when ψ is negative. To describe the saturation-pressure head relationship of unsaturated media, Mualem's model is used:

$$S = \frac{\theta - \theta_r}{\theta_s - \theta_r} = (1 + |\alpha\psi|^n)^{-m} \tag{2}$$

where θ is volumetric moisture content, θ_s is saturated moisture content, θ_r is moisture content at residual saturation and α, n, and m are fitting parameters where $m = 1 - 1/n$. This relationship leads to the following expression for the moisture capacity term, $C(\psi)$:

$$C(\psi) = \alpha(n-1)(\theta_s - \theta_r)S^{1/m}(1 - S^{1/m})^m \tag{3}$$

The unsaturated hydraulic conductivity is then given by:

$$K(\psi) = K_s\sqrt{S}(1 - (1 - S^{1/m})^m)^2 = K_s K_r \tag{4}$$

(van Genuchten, 1980) where K_s is saturated hydraulic conductivity. The dependence of these expressions on pressure is made explicit by substitution of (2). Based on these models the unsaturated hydraulic properties of a porous medium can be fully characterized if values of parameters, K_s, α, and n are specified. Hence, we are treating saturated hydraulic conductivity and the parameters α, and n as second-order stationary stochastic processes in space in order to represent heterogeneity of geological formations under unsaturated conditions. We further assume these stochastic processes are characterized by exponential covariance functions with known values of mean, variance, and correlation scale. An analysis of the relative conductivity and water retention of a large number of soil samples by Russo and Bouton (1992) gives some indication of the variance, anisotropy, and correlation scale of these parameters. However, in general, the covariance behavior of soil properties is site-specific and requires *a priori* evaluation. One approach to obtaining site-specific covariance behavior, which avoids detailed and extensive sampling by using all secondary as well as primary information, is the maximum likelihood estimation method developed by Kitanidis and Vomvoris (1983).

The saturated and residual moisture contents for this model are treated as deterministic constants based on the typically small variability of these parameters (Russo and Bouton, 1992). Incorporation of spatial variability in θ_s and θ_r into the model, however, is straightforward should it be important for a specific application.

Variability in pressure resulting from variability in K_s, α, and n is expressed to first-order by a Taylor series expansion

$$\psi = H + f\frac{\partial\psi}{\partial f}\bigg|_{H,F,A,N} + a\frac{\partial\psi}{\partial a}\bigg|_{H,F,A,N} + v\frac{\partial\psi}{\partial v}\bigg|_{H,F,A,N} \tag{5}$$

where the sensitivity derivatives are evaluated around the means, $H = E[\psi]$, $F = E[\ln(K_s)]$, $A = E[\ln(\alpha)]$, and $N = E[\ln(n)]$ and the zero mean perturbations are $f = F - \ln(K_s)$, $a = A - \ln(\alpha)$, $v = N - \ln(n)$, and $h = \psi - H$. Likewise a first-order Taylor series expansion of moisture content is

$$\theta = \Theta + f\frac{\partial\theta}{\partial f}\bigg|_{\Theta,F,A,N} + a\frac{\partial\theta}{\partial a}\bigg|_{\Theta,F,A,N} + v\frac{\partial\theta}{\partial v}\bigg|_{\Theta,F,A,N} \tag{6}$$

where $\Theta = E[\theta]$ and $\theta' = \theta - \Theta$.

Sensitivity derivatives in Eqs (5) and (6) are computed by the adjoint state sensitivity method (e.g., Sun and Yeh, 1992). Following the derivation of Li and Yeh (1998) the adjoint equation is

$$(\beta S_s + C(H))\frac{\partial \Phi}{\partial t} - K_s\frac{\partial K_r}{\partial \psi}\nabla(H+z)\nabla\Phi + \nabla\cdot(K_s K_r \nabla\Phi) = \delta(x - x_k, t - t_k) \tag{7}$$

where Φ is the adjoint state, subject to homogeneous boundary conditions and a homogeneous final condition at time $t = \tau_f$, δ is the Dirac delta function, and x_k and t_k are the space and time coordinates of a datum. Equation (7) is solved backwards in time to obtain $\Phi(t=0) = \Phi_0$ which is then used to derive the adjoint state, Φ^*, associated with the initial condition, based on the following equation:

$$K_s\frac{\partial K_r}{\partial \psi}\nabla(H+z)\nabla\Phi^* - \nabla\cdot(K_s K_r \nabla\Phi^*) = \Phi_0(\beta S_s + C(H)) \tag{8}$$

which is also subject to homogeneous boundary conditions. The sensitivity of head at location i to the change in f at location k is then

$$\frac{\partial \psi_i}{\partial f_k} = \int_0^{\tau_f}\int_{\Omega_k} K_s K_r \nabla(H+z)\nabla\Phi \,\mathrm{d}\Omega\,\mathrm{d}t + \int_{\Omega_k} K_s K_r \nabla(K+z)\nabla\Phi^* \,\mathrm{d}\Omega_k \tag{9}$$

where the space integral is only over the block or element, Ω_k, containing f_k. Using the same adjoint state variable, the sensitivity of head at location i to the change in a at location k is

$$\frac{\partial \psi_i}{\partial a_k} = \int_0^{\tau_f}\int_{\Omega_k} K_s\frac{\partial K_r}{\partial a}\nabla(H+z)\nabla\Phi \,\mathrm{d}\Omega\,\mathrm{d}t + \int_{\Omega_k} K_s\frac{\partial K_r}{\partial a}\nabla(H+z)\nabla\Phi^* \,\mathrm{d}\Omega_k \tag{10}$$

and to v is

$$\frac{\partial \psi_i}{\partial v_k} = \int_0^{\tau_f}\int_{\Omega_k} K_s\frac{\partial K_r}{\partial v}\nabla(H+z)\nabla\Phi \,\mathrm{d}\Omega\,\mathrm{d}t + \int_{\Omega_t} K_s\frac{\partial K_r}{\partial v}\nabla(H+z)\nabla\Phi^* \,\mathrm{d}\Omega_k \tag{11}$$

Sensitivity of moisture content to the variability of the K_s, α, and n, parameters can be obtained directly from sensitivities to pressure through equation (2) as

$$\frac{\partial \theta_i}{\partial f_k} = -\overline{m}(\theta_s - \theta_r)\left(1 + \left(-\overline{\alpha}H\right)^{\overline{n}}\right)^{-\overline{m}-1}\left(-\overline{\alpha}\,\overline{n}(-\overline{\alpha}H)^{\overline{n}-1}\right)\frac{\partial \psi_i}{\partial f_k} \tag{12}$$

$$\frac{\partial \theta_i}{\partial a_k} = -\overline{m}(\theta_s - \theta_r)\left(1 + (-\overline{\alpha}H)^{\overline{n}}\right)^{-\overline{m}-1}\overline{n}(\overline{\alpha}H)^{\overline{n}-1}\left(-\alpha\frac{\partial \psi_i}{\partial a_K} - H\right) \tag{13}$$

and

$$\frac{\partial \theta_i}{\partial v_k} = (\theta_s - \theta_r)\left[\frac{1}{\overline{n}^2}\left(1 + (-\overline{\alpha}H)^{\overline{n}}\right)^{\overline{m}} \ln\left(1 + (-\overline{\alpha}H)^{\overline{n}}\right)\frac{\partial \overline{n}}{\partial v}\right.$$
$$+ \left(\frac{1}{\overline{n}} - 1\right)\left(1 + (-\overline{\alpha}H)^{\overline{n}}\right)^{-m-1}(-\overline{\alpha}H)^{\overline{n}} \tag{14}$$
$$\left.\times \ln(-\overline{\alpha}H)\frac{\partial \overline{n}}{\partial v} - \overline{\alpha}\,\overline{n}(-\overline{\alpha}H)^{\overline{n}-1}\frac{\partial \psi_i}{\partial v_k}\right]$$

where $\partial\overline{n}/\partial v$ in Eq. (14) is one for v in the same block or element as θ_i and is zero otherwise. The bars over α, n and m indicate that the evaluation uses the geometric mean of these parameters.

Notice that one must derive the mean pressure head, H, first in order to evaluate the sensitivities discussed above. To do so, the mean equation is assumed to be the same as Richards equation, (1), and $K(\psi)$ and $C(\psi)$ are assumed to be described by Eqs (2)–(4) with parameter values set to their mean values (Yeh, 1998). Thus, the approximate mean pressure head can be obtained by solving

$$(\beta S_s + C(H))\frac{\partial H}{\partial t} = \nabla \cdot (K(H)\nabla(H + z)) \tag{15}$$

In this study, a finite element program (MMOC3) developed by Sravastava and Yeh (1992) was used to obtain the solution of (15) and (1) with heterogeneous parameters assumed constant across each element.

Once the mean pressure head is derived, the above sensitivity equations were used to calculate covariance and cross-covariances needed in our geostatistical approach. Discretizing the flow domain into n_e blocks or elements, multiplying Eqs (5) and (6) by perturbations f, a, and v and taking the expectation results in expressions for cross-covariance of head and moisture content with hydraulic properties as

$$\mathbf{R}_{hf} = \mathbf{R}_{ff}\mathbf{J}_{hf} \tag{16}$$
$$\mathbf{R}_{ha} = \mathbf{R}_{aa}\mathbf{J}_{ha} \tag{17}$$
$$\mathbf{R}_{hv} = \mathbf{R}_{vv}\mathbf{J}_{hv} \tag{18}$$
$$\mathbf{R}_{\theta' f} = \mathbf{R}_{ff}\mathbf{J}_{\theta' f} \tag{19}$$
$$\mathbf{R}_{\theta' a} = \mathbf{R}_{aa}\mathbf{J}_{\theta' a} \tag{20}$$

and

$$\mathbf{R}_{\theta' v} = \mathbf{R}_{vv}\mathbf{J}_{\theta' v} \tag{21}$$

In these expressions $\mathbf{R}_{ab}$ is notation for the covariance or cross-covariance matrix $E[\mathbf{ab}]$ where the subscripts refer to the zero mean perturbations defined above. The $n_e \times n_e$ matrices $\mathbf{R}_{ff}$, $\mathbf{R}_{aa}$, and $\mathbf{R}_{vv}$ are the assumed known input covariances of the log transformed perturbations of the hydraulic properties K_s, a, and n. Cross-covariance matrices $\mathbf{R}_{hf}, \mathbf{R}_{ha}, \mathbf{R}_{hv}, \mathbf{R}_{\theta' f}, \mathbf{R}_{\theta' a}$, and $\mathbf{R}_{\theta' v}$ have dimensions $n_e \times n_d$ where n_d is the number of head or moisture content data locations. The matrices $\mathbf{J}_{hf}, \mathbf{J}_{ha}, \mathbf{J}_{hv}, \mathbf{J}_{\theta' f}, \mathbf{J}_{\theta' a}$, and $\mathbf{J}_{\theta' v}$ also are $n_e \times n_d$ and are obtained from Eqs. (9–14) at the sample locations $i = 1, \ldots, n_d$. In the formulation of

Eqs. (16–21) we have assumed that the hydraulic properties K_s, a, and n are independent since no sufficient data set is available to quantify their cross-correlation. Note that our assumption of independence represents the worst case, meaning that information about one parameter tells us nothing about the others.

Covariances of the perturbations in pressure, h, and moisture content, θ', are derived by multiplying Eqs (5) and (6) by the perturbations, taking the expectation, and substituting Eqs (16–21) as

$$\mathbf{R}_{hh} = \mathbf{J}_{hf}^{\mathrm{T}}\mathbf{R}_{ff}\mathbf{J}_{hf} + \mathbf{J}_{ha}^{\mathrm{T}}\mathbf{R}_{aa}\mathbf{J}_{ha} + \mathbf{J}_{hv}^{\mathrm{T}}\mathbf{R}_{vv}\mathbf{J}_{hv} \tag{22}$$

$$\mathbf{R}_{\theta'\theta'} = \mathbf{J}_{\theta'f}^{\mathrm{T}}\mathbf{R}_{ff}\mathbf{J}_{\theta'f} + \mathbf{J}_{\theta'a}^{\mathrm{T}}\mathbf{R}_{aa}\mathbf{J}_{\theta'a} + \mathbf{J}_{\theta'v}^{\mathrm{T}}\mathbf{R}_{vv}\mathbf{J}_{\theta'v} \tag{23}$$

The cross-covariance function between h and θ' is given by

$$\mathbf{R}_{h\theta'} = \mathbf{J}_{hf}^{\mathrm{T}}\mathbf{R}_{ff}\mathbf{J}_{\theta'f} + \mathbf{J}_{ha}^{\mathrm{T}}\mathbf{R}_{aa}\mathbf{J}_{\theta'a} + \mathbf{J}_{h}v^{\mathrm{T}}\mathbf{R}_{vv}\mathbf{J}_{\theta'v} \tag{24}$$

In the aforementioned equations, T indicates transpose. Note that a second-order approximation of these covariances can be obtained by the method developed by Liedl (1994).

A first-order estimate of the perturbations in the log-transformed hydraulic properties, which matches data of the hydraulic property of interest and incorporates secondary information, can be obtained from the classical cokriging technique which involves solving the equations

$$\begin{bmatrix} \mathbf{C}_{ff} & \mathbf{C}_{fa} & \mathbf{C}_{fv} & \mathbf{C}_{\theta'f} & \mathbf{C}_{hf} \\ \mathbf{C}_{fa}^{T} & \mathbf{C}_{aa} & \mathbf{C}_{av} & \mathbf{C}_{\theta'a} & \mathbf{C}_{ha} \\ \mathbf{C}_{fv}^{T} & \mathbf{C}_{av}^{T} & \mathbf{C}_{vv} & \mathbf{C}_{\theta'v} & \mathbf{C}_{hv} \\ \mathbf{C}_{\theta'f}^{T} & \mathbf{C}_{\theta'a}^{T} & \mathbf{C}_{\theta'v}^{T} & \mathbf{C}_{\theta'\theta'} & \mathbf{C}_{h\theta'} \\ \mathbf{C}_{hf}^{T} & \mathbf{C}_{ha}^{T} & \mathbf{C}_{hv}^{T} & \mathbf{C}_{h\theta'}^{T} & \mathbf{C}_{hh} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}_f \\ \boldsymbol{\lambda}_a \\ \boldsymbol{\lambda}_v \\ \boldsymbol{\lambda}_{\theta'} \\ \boldsymbol{\lambda}_h \end{bmatrix} = \begin{bmatrix} \mathbf{C}_{f\chi} \\ \mathbf{C}_{a\chi} \\ \mathbf{C}_{v\chi} \\ \mathbf{C}_{\theta'\chi} \\ \mathbf{C}_{h\chi} \end{bmatrix} \tag{25}$$

In this matrix formulation of the cokriging eqs. $\mathbf{C}_{ff}, \mathbf{C}_{\theta'f}, \mathbf{C}_{hf}, \mathbf{C}_{aa}, \mathbf{C}_{\theta'a}, \mathbf{C}_{ha}, \mathbf{C}_{vv}, \mathbf{C}_{\theta'v}, \mathbf{C}_{hv}, \mathbf{C}_{\theta'\theta'}, \mathbf{C}_{h\theta'}$, and $\mathbf{C}_{hh}$ represent covariances and cross-covariances of the data locations, which are subsets of covariance and cross-covariance matrices obtained from Eqs. (16–24). Under our assumption of hydraulic property independence, $\mathbf{C}_{fa}, \mathbf{C}_{fv}$, and $\mathbf{C}_{av}$ are matrices of zeros. The matrices $\boldsymbol{\lambda}_f, \boldsymbol{\lambda}_a, \boldsymbol{\lambda}_v, \boldsymbol{\lambda}_{\theta'}$, and $\boldsymbol{\lambda}_h$ are the cokriging weights applied to data of K_{s}, a, n, moisture content, and pressure. On the right hand side are the covariances and cross-covariances of the data locations with the location to be estimated. Covariances on the right hand side of Eq. (25) are matrices with the number of data, $K_{\mathrm{s}}, a, n, \theta$, or p rows and n_{e} columns and the cokriging weights are also matrices of the same dimensions. Once the weights are evaluated, linear estimates of the hydraulic properties given data vectors $\mathbf{f}_{\mathrm{d}}, \mathbf{a}_{\mathrm{d}}, \boldsymbol{v}_{\mathrm{d}}, \boldsymbol{\theta}'_{\mathrm{d}}$, and $\mathbf{h}_{\mathrm{d}}$ are

$$f = \boldsymbol{\lambda}_f^T\mathbf{f}_{\mathrm{d}} + \boldsymbol{\lambda}_a^T\mathbf{a}_{\mathrm{d}} + \boldsymbol{\lambda}_v^T v_{\mathrm{d}} + \boldsymbol{\lambda}_{\theta'}^T\theta'_{\mathrm{d}} + \boldsymbol{\lambda}_h^T\mathbf{h}_{\mathrm{d}} \tag{26}$$

$$a = \boldsymbol{\lambda}_f^T\mathbf{f}_{\mathrm{d}} + \boldsymbol{\lambda}_a^T\mathbf{a}_{\mathrm{d}} + \boldsymbol{\lambda}_v^T v_{\mathrm{d}} + \boldsymbol{\lambda}_{\theta'}^T\theta'_{\mathrm{d}} + \boldsymbol{\lambda}_h^T\mathbf{h}_{\mathrm{d}} \tag{27}$$

and

$$v = \boldsymbol{\lambda}_f^T\mathbf{f}_{\mathrm{d}} + \boldsymbol{\lambda}_a^T\mathbf{a}_{\mathrm{d}} + \boldsymbol{\lambda}_v^T v_{\mathrm{d}} + \boldsymbol{\lambda}_{\theta'}^T\theta'_{\mathrm{d}} + \boldsymbol{\lambda}_h^T\mathbf{h}_{\mathrm{d}} \tag{28}$$

for χ equal f, a, or v in Eq. (25). The vectors $f_{\mathrm{d}}, a_{\mathrm{d}}, \mathbf{v}_{\mathrm{d}}$, $\boldsymbol{\theta}'_{\mathrm{d}}$, and h_{d} are data of perturbations in ln K_s, ln a, ln n, moisture content, and pressure. The $n_{\mathrm{e}} \times 1$ vectors **f**, **a**, and v are estimates of the perturbations in ln K_s, ln a, ln n.

3 Numerical examples

3.1 1-D flow

To verify the geostatistical inversion method a one-dimensional steady infiltration problem is used. The one-dimensional flow domain is a vertical column 64 cm in height discretized into 64 cubic elements 1 cm on each side. Boundary conditions are prescribed pressure at the top and bottom of the column and no-flow perpendicular to the sides. Three unit gradient flow scenarios involving three different top and bottom boundary conditions were examined. That is, pressures at the top and bottom of the column were set equally to -5, and -50, and -300 cm for the three cases to reflect nearly saturated and drier mean flow conditions. The geometric mean of saturated hydraulic conductivity of the porous medium of the domain is 2.694×10^{-4} cm/s and the geometric means of α and n parameters are $0.0136\,\mathrm{cm}^{-1}$ and 2.3543 respectively. Saturated moisture content of 0.37 and residual moisture content of 0.06 are presumed known and deterministic. Variance of f is 0.0215, variance of a is 0.0660, and variance of v is 0.0079. All three variable parameters have a correlation length of 12 cm in the vertical direction. Random fields of f, a, and v, were generated by the spectral method (Gutjahr, 1989). With the random fields as input, MMOC3 (Sravastava and Yeh, 1992) was used to compute head and moisture content distributions along the flow domain. Perturbations in head and moisture content were then obtained by subtracting the mean head and moisture content from their corresponding fields in the heterogeneous domain. The mean fields were obtained from the solution to the approximate mean flow Eq. (15).

Three fully determined (or deterministic, Yeh et al., 1996) inverse problems associated with the one-dimensional flow geometry are used to test our inverse algorithm. Under saturated steady flow situations, the inverse problem is fully determined if all the heads and boundary fluxes are known precisely with no measurement error. For the unsaturated flow problem examined here, the inverse problem will be unique if either all the heads or moisture contents and the distributions of two of the three parameters are known perfectly. The inverse problem is also unique if one of the three parameter fields is known in addition to the information about all heads and all moisture contents. For these problems, any good inverse model should identify the unknown parameter field with a reasonable accuracy. This is the objective of our test.

Figure 1a compares, at a uniform mean pressure of -5 cm, the true f field with our estimate using all head data and 1 f sample. In this example the a and v fields are assumed to be zero, i.e. parameters α and n are represented as constants equal to their geometric means. Figure 1b compares the true a field with the estimated field based on 64 θ data, and one a value, at a uniform mean pressure of -50 cm, where f and v are known. The comparison of the true v field with the estimate using 64 θ data and 1 v datum, at a uniform mean pressure of -300 cm, is shown in Fig. 1c where f and a are known.

The estimated f field using 64 head samples, 64 measurements of θ (at a uniform mean pressure of -5 cm),and one measurement each of f and a is shown compared to the true field in Fig. 2a. In this example both f and a are random

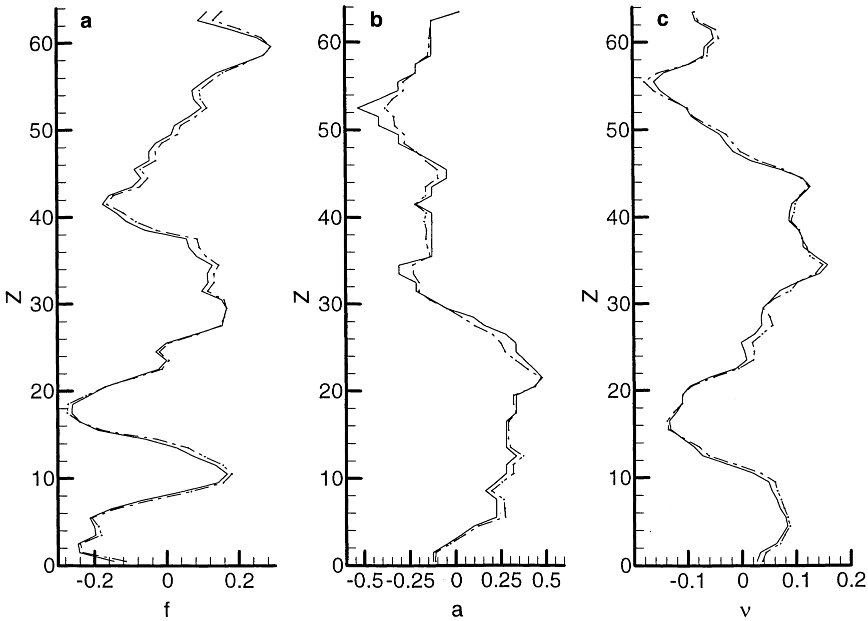

Fig. 1. Fully determined 1-D inverse estimates of: **a**) f using 64 h data and 1 f datum at mean pressure -5 cm where α and n are constants, **b**) a using 64 θ and 1 a at mean pressure -50 cm where K_s and n are constants, and **c**) ν using 64 θ data and 1 ν at mean pressure -300 cm where K_s and α are constants. The true field is indicated by a solid line and the estimate is shown as a dashed line

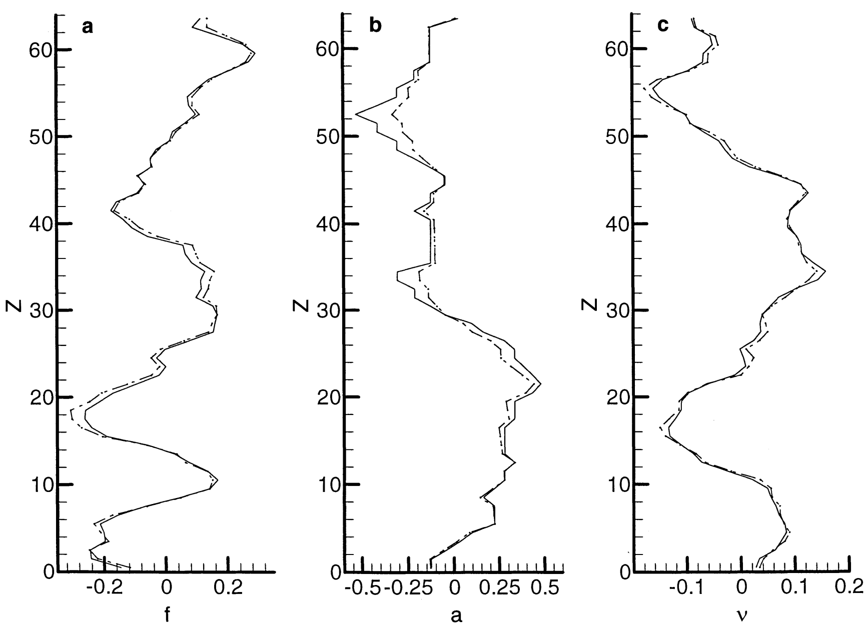

Fig. 2. Fully determined 1-D inverse estimates of: **a**) f using 64 h, 64 θ, 1 f, and 1 a at mean pressure -5 cm where n is constant, **b**) a using 64 h, 64 θ, 1 f, and 1 a at mean pressure -50 cm where n is constant, and **c**) ν using 64 h, 64 θ, 1 f, and 1 ν at mean pressure -300 cm where α is constant. The true field is indicated by a solid line and the estimate is shown as a dashed line

fields and v is an assumed known constant. In Fig. 2b, a is estimated using 64 h, 64 θ, 1 f, and 1 a at a mean pressure of -50 cm where, again, both f and a are random and v is known. Parameters a and v are variable and f is held constant in Figure 2c while v is estimated using 64 h, 64 θ, 1 v, and 1 a at a mean pressure of -300 cm. In all cases the geostatistical estimation procedure produces an accurate depiction of the true underlying variable parameter fields for the fully determined inverse problem.

Correlation between parameters and the system response in terms of pressure and moisture content perturbations is a function of the mean pressure. Figure 3 shows the cross-correlation between parameters and pressure and moisture content perturbations, at a location 29.5 cm from the base of the column. Cross-correlation with f is shown in Fig. 3a, with a in Fig. 3b, and with v in Fig. 3c at pressures of $-5, -50$, and -300 cm. Correlation at a mean pressure of -5 cm is indicated by a solid line, correlation at a mean pressure of -50 cm by a dashed line, and correlation at a mean pressure of -300 cm by a dotted line. Correlation between perturbations in parameters and moisture content are further denoted by small dot symbols while correlation between parameter perturbations and pressure is shown as lines without symbols. Figure 3 shows that pressure perturbations are more strongly correlated with perturbations in the log of saturated hydraulic conductivity near saturation. Correlation of both moisture content and pressure perturbations with a appears to increase from a mean pressure of -5 to -50 cm then decrease from -50 to -300 cm. A similar behavior can be seen in the correlation of v with both h and θ in Fig. 3c except that the correlation between v and θ is positive at a mean pressure of -5 cm and negative at a mean pressure of -300 cm.

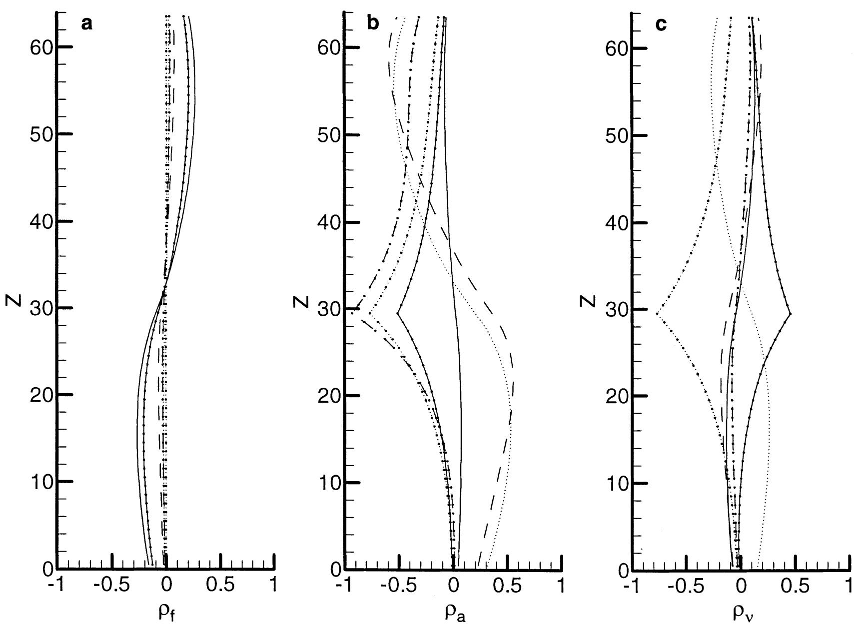

Fig. 3. Correlation of pressure and moisture content at $z = 29.5$ cm with **a**) f, **b**) a, and **c**) v. Solid line indicates correlation at mean pressure -5 cm, dashed line indicates correlation at mean pressure -50 cm, and dotted line indicates correlation at mean pressure -300 cm. Correlation between moisture content and parameters is indicated with small dot symbols while correlation between pressure and parameters is indicated by lines without symbols

3.2
3-D flow

After testing our inverse model we applied it to a 3-dimensional steady state flow problem. The three-dimensional flow domain is discretized into 6 nodes in the x direction, 6 nodes in the y direction, and 21 nodes in the z direction for a total of 756 nodes and 500 elements. Note that in a finite element formulation pressure and moisture contents are defined at the nodes while model parameters are defined over the element. To resolve this for the inverse solution, pressure and moisture content for an element were obtained as the arithmetic average of the values at the nodes of an element. The spacing between nodes is a uniform 0.4 m in the x and y directions and 0.1 m in the z direction resulting in a cubic domain 2 m on each side. Boundary conditions along the bottom at $z = 0$ m are a prescribed constant pressure of 10 m for saturated flow and -2 m for unsaturated flow conditions. Boundary conditions perpendicular to all four sides are no-flow. At the surface of the domain, $z = 2$ m, a prescribed head boundary is specified in the central region from 0.8 m $\leq x \leq$ 1.2 m and 0.8 $m \leq y \leq$ 1.2 m while the remainder of the top surface is treated as a no-flow boundary. Three flow regimes were studied: Case 1 represents flow under a fully saturated condition where a pressure head of 10 m is specified for the top prescribed head boundary, Case 2 uses prescribed pressure boundary conditions of -0.1 m at the top and -2 m at the bottom to represent unsaturated flow at wetter conditions, and Case 3 uses -2 m at both top and bottom for unsaturated flow at drier conditions. Parameters (K_s, α and n) are assumed to be spatial stochastic processes in three-dimensions. Geometric means of these parameters are 0.234 m/hr for K_s, 0.4233/m for α, and 2.0594 for n, which correspond to the properties of a silt loam (Stephens et al., 1987). Variance of the logarithm of perturbations in these parameters are 0.0189 for f, 0.0213 for a, and 0.0024 for v. Correlation structures of all three random parameters are assumed exponential with a correlation scale of 6 m in the x and y directions and 1.5 m in the z direction. Water content at saturation θ_s and residual water content θ_r are assumed constant in space and set to values of 0.43 and 0.1313, respectively. Seven well locations, shown in map view in Fig. 4, were sampled at depths of 0.15, 0.45, 0.75, 1.05, 1.35, and 1.65 m for a total of 42 samples. Data of the primary variables, one each of K_s, α, and n are located at the 0.75 m depth of the center well.

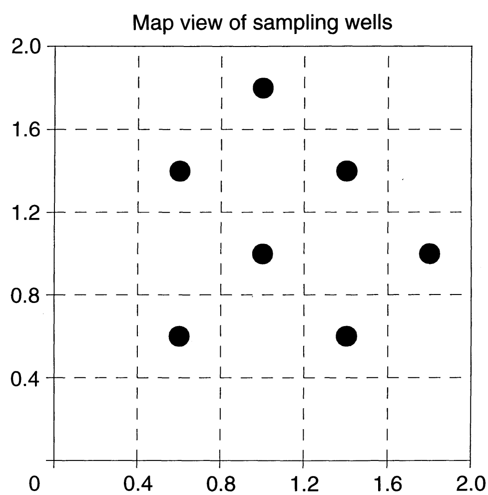

Fig. 4. Map view of the surface of the 3-D domain showing sampling well locations.

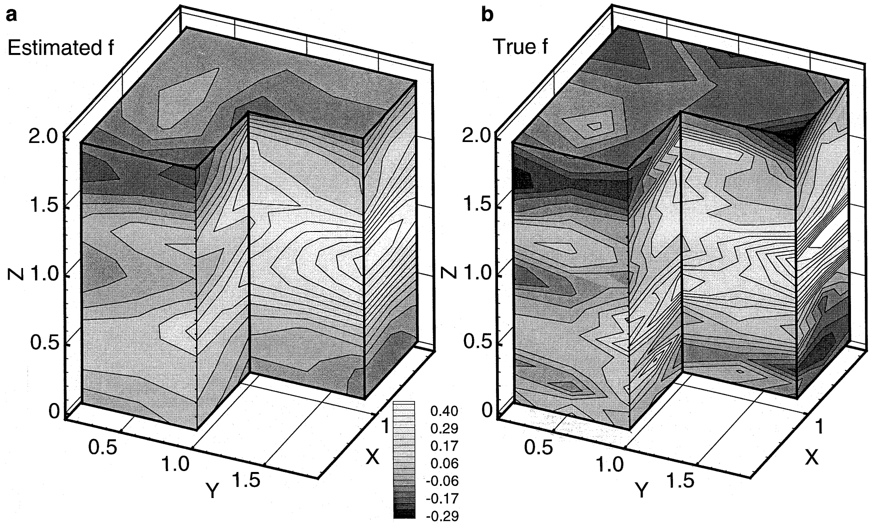

Fig. 5. a) f field estimated using 42 h, 1 f, 1 a, and 1 ν data under saturated flow conditions. **b)** True f field.

The estimate of the f field using 42 pressure perturbation data for Case 1 is shown in Fig. 5a. Compared with the true f field shown in Fig. 5b, much of the detail of the true f parameter is revealed in our estimate due to the high correlation between f and h in this case. An estimate of the a field using 42 moisture content data of Case 2 is shown in Fig. 6a compared to the true a field shown in Fig. 6b. Boundary conditions of -0.1 m at the central region of the top and -2 m along the bottom produce relatively moist unsaturated flow at which moisture content and the a parameter are highly correlated. Thus significant information

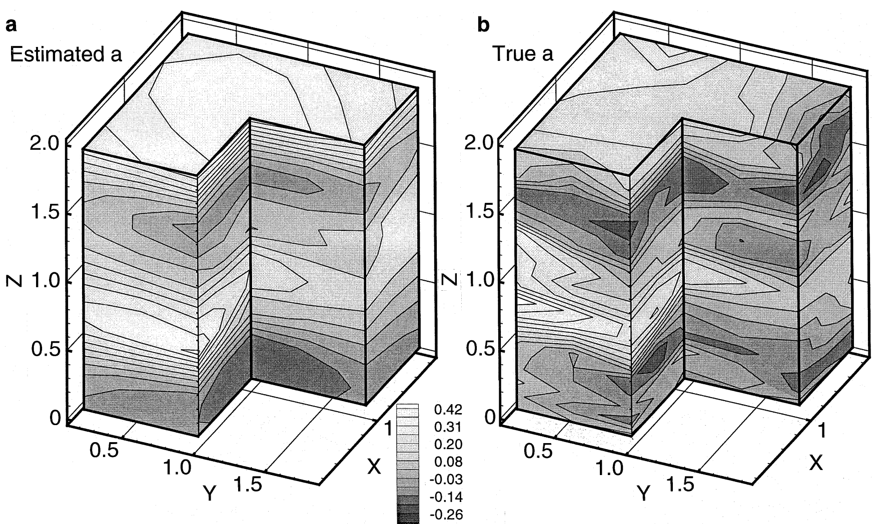

Fig. 6. a) a field estimated using 42 θ, 1 f, 1 a, and 1 ν data for unsaturated flow conditions with top boundary set to -0.1 m and bottom boundary -2 m. **b)** True a field

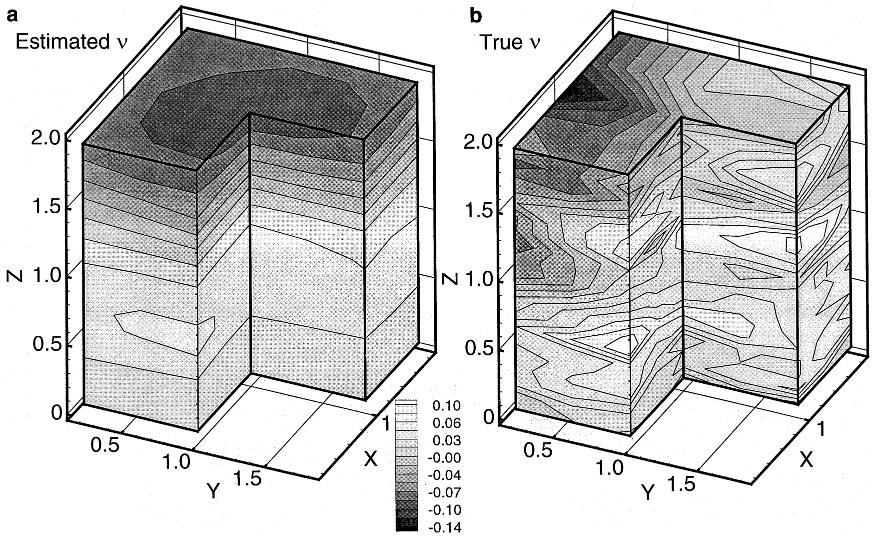

Fig. 7. a) ν field estimated using 42 θ, 1 f, 1 a, and 1 ν data for unsaturated flow conditions with top boundary set to −2 m and bottom boundary −2 m. **b)** True ν field

regarding the α parameter is obtained from moisture content data. An estimate of v using 42 moisture content data under drier unsaturated flow conditions (Case 3) is shown in Fig. 7a and the true v field is shown in Fig. 7b. While the correlation between moisture content and v is stronger for drier unsaturated conditions than for wetter conditions, only the general trend of the v field and very little of the detail is revealed by the moisture content data.

Figure 8 shows the correlation between the f, a, and v fields, along the axis of the central sampling well, with a pressure or moisture content perturbation at $z = 0.95$ m. A strong correlation between the perturbations in pressure and the log of saturated hydraulic conductivity occurs under saturated flow conditions (Fig. 8a). Likewise a strong correlation between moisture content perturbations and the log of the α parameter is seen in unsaturated flow. This correlation explains the fairly accurate estimation of f and a seen in Figs 5 and 6. Correlation is a good indication of estimation accuracy here because the variance is small and thus the linear approximation is adequate. A weaker correlation exists between moisture content or pressure perturbations and the log of the n parameter (Fig. 8c). This accounts for the poorer estimation of the v field as seen in Fig. 8c. Also, the linear assumption inherent in the cokriging estimator is probably less accurate since the n parameter appears in the exponent of the van Genuchten model.

4
Discussion and summary

Accurate geostatistical estimation of the hydraulic properties of unsaturated flow is possible using data of pressure and moisture content as long as the variances of the hydraulic properties are small enough so that a linear approximation is valid. For higher variances it is possible to incorporate nonlinearities through an iterative approach. Results of the iterative improvement of estimates for higher variance cases will be presented in a subsequent paper. In this analysis it is seen

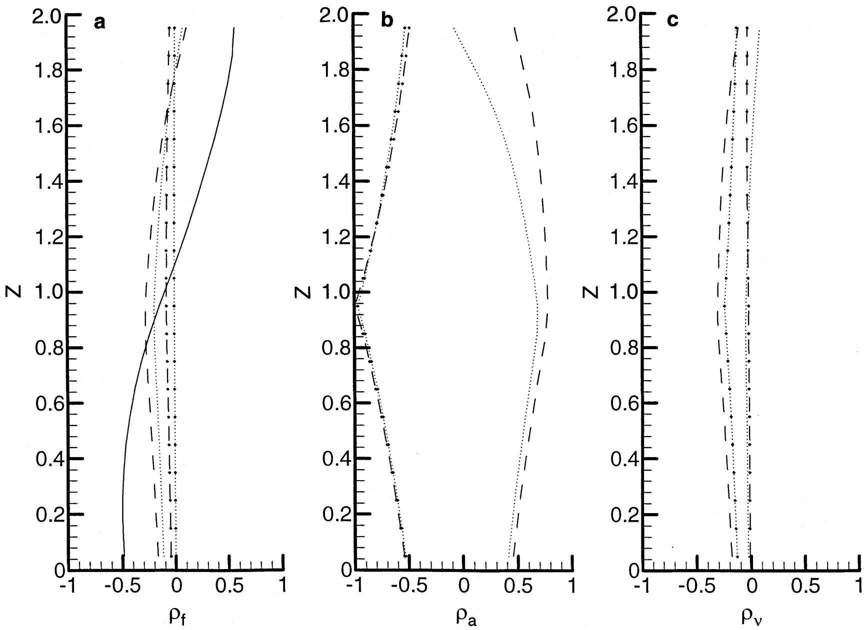

Fig. 8. Correlation of pressure and moisture content at $x = 1$ m, $y = 1$ m, $z = 0.95$ m with **a**) f, **b**) a, and **c**) ν on a vertical transect along the axis of the central well. Solid line indicates correlation at saturated flow conditions, dashed line indicates correlation at unsaturated flow conditions with the top boundary -0.1 m and the bottom boundary -2 m, and dotted line indicates correlation at unsaturated flow conditions with the top boundary -2 m and the bottom boundary -2 m. Correlation between moisture content and parameters is indicated with small dot symbols while correlation between pressure and parameters is indicated by lines without symbols

that correlation between parameters and system state is highly dependent on mean pressure or saturation. This information is useful in the design of sampling programs as it indicates the relative "worth" of secondary information in the estimation process. Thus the modeling can be used to direct the most efficient and cost-effective site characterization efforts.

We developed a three-dimensional variably saturated inverse flow model for estimating, to first-order, perturbations in the log-transformed α and n parameters of the van Genuchten soil moisture – hydraulic conductivity relationship and the log-transformed saturated hydraulic conductivity using pressure and moisture content data. The model appears to be insensitive to the relationship between the correlation scale of the parameter heterogeneity and the size of the domain. Good results were obtained in the 1-D case where the flow domain was a multiple of the correlation scale and in the 3-D case where the correlation scale was a multiple of the domain size. The preliminary results presented here for estimating heterogeneous hydraulic properties, using easily measured moisture content and pressure data, demonstrate the promise of the geostatistical inverse technique for identifying vadose zone model parameters.

References

Gutjahr A (1989) Fast Fourier transforms for random field generation. N.M. Tech Project Report: 106 pp

Kitanidis PK, Vomvoris EG (1983) A geostatistical approach to the inverse problem in groundwater modeling (steady state) and one-dimensional simulations. Water Resour. Res. 19: 677–690

Li B, Yeh T-C (1998) Sensitivity and moment analyses of head invariably saturated flow regimes. Adv. Water Resour. 21: 477–485

Liedl R (1994) A conceptual perturbation model of water movement in stochastically heterogeneous soils. Adv. Water Resour. 17: 171–179

Russo D, Bouton M (1992) Statistical analysis of spatial variability in unsaturated flow parameters. Water Resour. Res. 28(7): 1911–1925

Sravastava R, Yeh T-C (1992) A three-dimensional numerical model for water flow and transport of chemically reactive solute through porous media under variably saturated conditions. Adv. Water Resour. 15(5): 275–287

Stephens DB, Lambert K, Watson D (1987) Regression models for hydraulic conductivity and field test of the bore hole permeameter. Water Resour. Res. 23(12): 2207–2214

Sun N-Z, Yeh WW-G (1992) A stochastic inverse solution for transient groundwater flow: parameter identification and reliability analysis. Water Resour. Res. 28(12): 3269–3280

van Genuchten MT (1980) A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. 44: 892–898

Yeh T-C (1998) Scale issues of heterogeneity in vadose-zone hydrology and practical solutions, in Scale Dependence and Scale Invariance in Hydrology, edited by G. Sposito, Cambridge Press (in print)

Yeh T-C, Jin M, Hanna S (1996) An iterative stochastic inverse method: conditional effective transmissivity and hydraulic head fields. Water Resour. Res. 32(1): 85–92

Yeh T-C, Zhang J (1996) A geostatistical inverse method for variably saturated flow in the vadose zone, Water Resour. Res. 32(9): 2757–2766

Zhang J, Yeh T-C (1997) An iterative geostatistical inverse method for steady flow in the vadose zone. Water Resour. Res. 33(1): 63–71