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A geostatistical inverse method for variably saturated flow in the vadose zone

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Abstract. A geostatistical inverse technique utilizing both primary and secondary information is developed to estimate conditional means of unsaturated hydraulic conductivity parameters (saturated hydraulic conductivity and pore size distribution parameters) in the vadose zone. Measurements of saturated hydraulic conductivity and pore size distribution parameters are considered as the primary information, while measurements of steady state flow processes (soil-water pressure head and degree of saturation) are regarded as the secondary information. This inverse approach relies on the classical linear predictor (cokriging) theory and takes the advantage of the spatial cross correlation between the soil-water pressure head and each of the following: degree of saturation, saturated hydraulic conductivity, and a pore size distribution parameter. Using an approximate perturbation solution for steady, variably saturated flow under general boundary conditions, the cross covariances between the primary and secondary information are derived. The approximate solution is formulated on the basis of a first-order Taylor series expansion of a discretized finite element equation. The sensitivity matrix in the solution is evaluated by an adjoint state sensitivity approach for flow in heterogeneous media under variably saturated conditions. Through several numerical examples the inverse model demonstrates its ability to improve the estimates of the spatial distribution of saturated hydraulic conductivity and pore size distribution parameters using the secondary information.

Introduction

The cokriging technique has been widely adopted to estimate transmissivity, head, velocity, and concentration of pollutants in aquifers [*Kitanidis and Vomvoris*, 1983; *Hoeksema and Kitanidis*, 1984, 1989; *Rubin and Dagan*, 1987; *Gutjahr and Wilson*, 1989; *Harvey and Gorelick*, 1995; *Yeh et al*., 1995a, 1996]. It has also been applied to estimate water content in the vadose zone, using water content, soil-water pressure head, soil surface temperature, and soil texture data sets [e.g., *Vauclin et al*., 1983; *Yates and Warrick*, 1987; *Mulla*, 1988]. However, little attention has been directed toward the application of this method to the inverse problem in the vadose zone (i.e., estimation of unsaturated hydraulic conductivity parameters using soil-water pressure head and water content data sets).

Predicting water and solute movements in the vadose zone with a reasonable accuracy requires a large number of measurements of the unsaturated hydraulic conductivity [e.g., *Yeh and McCord*, 1994; *Yeh*, 1995]. Unlike saturated hydraulic conductivity, the hydraulic conductivity of unsaturated porous media is a nonlinear function of soil-water pressure head and moisture content. Because of this nonlinearity, measurements of the unsaturated hydraulic conductivity are thus a difficult, time-consuming, and costly task. Subsequently, characterization of the vadose zone by direct measurements of the hydraulic conductivity at a large number of locations becomes a formidable task. On the other hand, information about flow processes such as soil-water pressure head and water content data sets can be collected with relative ease in most shallow and unconsolidated vadose zones with inexpensive tools. Water content data sets may, however, be the only information that can be collected in large quantities in the thick vadose zone of the western region of United States. Poorly sorted alluvial deposits, conglomerates, and solid rock masses composing the vadose zone in the region often prohibit the use of pressure measurement devices. As a result, it seems logical to take advantage of the abundance of information about flow processes to improve our estimates of unsaturated hydraulic properties in the field. In fact, *Harter and Yeh* [1996] recently demonstrated that using cokriging and a numerical model with a large amount of soil-water pressure head measurements can greatly improve the prediction of movement of solutes in the vadose zone. While their finding is promising, the method is limited to unit mean gradient, uniform flow, and stationary conditions which may not be suitable for application to a wide range of field problems.

In this paper a flexible geostatistical inverse technique that can utilize both soil-water pressure and water content data sets is developed to estimate the approximate conditional mean unsaturated hydraulic conductivity parameters in the vadose zone. The technique is flexible in the sense that it can be applied to nonuniform flow and nonstationary problems under field conditions. To demonstrate the ability of the proposed methodology and the benefit of using soil-water pressure head and water content to estimate the unsaturated hydraulic conductivity parameters, several numerical experiments were carried out. Explanations for the improvement on the estimates due to the use of both soil-water pressure and water content data sets are provided.

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Mathematical Formulations

Governing Flow Equations

Steady state flow in two-dimensional heterogeneous porous media under variably saturated conditions can generally be described by

$$\frac{\partial}{\partial x_i}\left[K(\psi)\frac{\partial(\psi+x_2)}{\partial x_i}\right]=0 \qquad i=1,2 \tag{1}$$

with specified boundary conditions

$$\begin{aligned}\psi &= \psi^* \qquad \text{on } \Gamma_1\\ q_i n_i &= q^* \qquad \text{on } \Gamma_2\end{aligned} \tag{2}$$

where x_1 and x_2 are horizontal and vertical coordinates (positive upward), respectively. The soil-water pressure head, ψ, is positive for saturated flow and negative for unsaturated flow. The prescribed head on boundary Γ_1 is ψ^*, and q^* is the prescribed flux normal to boundary Γ_2. $K(\psi)$ is the unsaturated hydraulic conductivity (assumed locally isotropic), which varies with ψ under unsaturated conditions. In this study the Gardner-Russo model [*Russo*, 1988] is used to describe the relationship between K and ψ. That is,

$$K(\psi,\mathbf{x})=K_s(\mathbf{x})\exp\left[\alpha(\mathbf{x})\psi(\mathbf{x})\right] \tag{3}$$

where $\mathbf{x}$ is the position vector, $\{x_1, x_2\}$, K_s is the saturated hydraulic conductivity, and α is a pore size distribution parameter. The relationship between water content and soil-water pressure head is described by the following function:

$$\Theta=\frac{\theta-\theta_r}{\theta_s-\theta_r}=e^{-0.5\alpha|\psi|}(1+0.5\alpha|\psi|)^{2/\tau+2} \tag{4}$$

where Θ is degree of saturation or effective saturation, θ is the moisture content, θ_s and θ_r are saturated and residual moisture contents, respectively, and τ is a soil parameter which accounts for the tortuosity of the flow path and the correlation between pores.

Geostatistical Inverse Approach

Assume that the natural log of saturated hydraulic conductivity ln K_s and pore size distribution coefficient ln α are stochastic processes with means E[ln K_s] $= F(x)$ and E[ln α] $= A(x)$ and perturbations $f(x)$ and $a(x)$, respectively. Similarly, the soil-water pressure ψ and effective saturation Θ are also considered as stochastic processes that can be expressed as $\psi(x) = H(x) + h(x)$ and $\Theta(x) = S(x) + s(x)$, where $H(x) = E[\psi(x)]$ and $S(x) = \mathrm{E}[\Theta(x)]$ are the means and $h(x)$ and $s(x)$ are the perturbations, respectively. Suppose we have n_f observed saturated hydraulic conductivities $f(x_i)$, where $i = 1, 2, \cdots, n_f$; n_a observed pore size distribution coefficient $a(x_j)$, where $j = 1, 2, \cdots, n_a$; n_h soil-water pressure measurements, $h(x_k)$, where $k = 1, 2, \cdots, n_h$; and n_s sampled effective saturation $s(x_l)$, where $l = 1, 2, \cdots, n_s$. We want to estimate f and a at locations where no samples are available. In the stochastic concept, one desirable estimate is the fields of f and a that represent the realizations conditioned on the measurements. The other is the expected value of all the possible realizations of f and a fields that are conditioned on the measurements of f, a, h, and s (conditional means). Theoretically, the former will have an infinite number of possibilities and the latter is unique. Our geostatistical inverse approach is intended to derive the conditional mean fields.

If we assume that the distributions of f, a, h, and s are jointly normal, the conditional mean estimates of $f(x)$ and $a(x)$ at unsampled locations $\mathbf{x}_0$ can be expressed by the linear combination of the weighted observed values of f, a, h, and s (assuming f and a are uncorrelated).

$$\begin{aligned}f_{co}(\mathbf{x}_0)&=\sum_{i=1}^{n_f}P_{fi}f(\mathbf{x}_i)+\sum_{k=1}^{n_h}Q_{fk}h(\mathbf{x}_k)+\sum_{l=1}^{n_s}R_{fl}s(\mathbf{x}_l)\\ a_{co}(\mathbf{x}_0)&=\sum_{j=1}^{n_a}P_{aj}a(\mathbf{x}_j)+\sum_{k=1}^{n_h}Q_{ak}h(\mathbf{x}_k)+\sum_{l=1}^{n_s}R_{al}s(\mathbf{x}_l)\end{aligned} \tag{5}$$

In (5), f_{co} and a_{co} are the cokriged values of f and a at the unsampled location, $\mathbf{x}_0$. P_{fi}, Q_{fk}, and R_{fl} are cokriging coefficients for estimation of f with respect to the measurements of f, h, and s; P_{aj}, Q_{ak}, and R_{al} are cokriging coefficients for the estimate of a with respect to the samples of a, h, and s. The i, j, k, and l are the indices for observed f, a, h, and s, respectively. These cokriging coefficients are selected in such a way that the estimations expressed by (5) will have the minimal variances, or

$$\begin{aligned}E[(f_{co}-f^*)^2]&=\min\\ E[(a_{co}-a^*)^2]&=\min\end{aligned} \tag{6}$$

where f^* and a^* are the unknown true values of f and a at the unsampled location.

Substituting (5) into (6), taking the derivatives of (6) with respect to the coefficients, and setting the resultants to zero lead to two sets of the cokriging system of equations. The cokriging system of equations for calculating the cokriging coefficients related to saturated hydraulic conductivity, P_{fI}, Q_{fk}, and R_{fl}, are

$$\begin{aligned}&\sum_{mi=1}^{n_f}P_{fi}C_{ff}(\mathbf{x}_i,\mathbf{x}_{mi})+\sum_{mk=1}^{n_h}Q_{fk}C_{fh}(\mathbf{x}_i,\mathbf{x}_{mk})+\sum_{ml=1}^{n_s}R_{fl}C_{fs}(\mathbf{x}_i,\mathbf{x}_{ml})\\ &\qquad=C_{ff}(\mathbf{x}_i,\mathbf{x}_0)\\ &\sum_{mi=1}^{n_f}P_{fi}C_{hf}(\mathbf{x}_k,\mathbf{x}_{mi})+\sum_{mk=1}^{n_h}Q_{fk}C_{hh}(\mathbf{x}_k,\mathbf{x}_{mk})+\sum_{ml=1}^{n_s}R_{fl}C_{hs}(\mathbf{x}_k,\mathbf{x}_{ml})\\ &\qquad=C_{hf}(\mathbf{x}_k,\mathbf{x}_0)\\ &\sum_{mi=1}^{n_f}P_{fi}C_{sf}(\mathbf{x}_l,\mathbf{x}_{mi})+\sum_{mk=1}^{n_h}Q_{fk}C_{sh}(\mathbf{x}_l,\mathbf{x}_{mk})+\sum_{ml=1}^{n_s}R_{fl}C_{ss}(\mathbf{x}_l,\mathbf{x}_{ml})\\ &\qquad=C_{sf}(\mathbf{x}_l,\mathbf{x}_0)\end{aligned} \tag{7}$$

The cokriging coefficients associated with pore-size distribution parameter, P_{aI}, Q_{ak}, and R_{aI}, can be derived by solving the other set of the system of equations:

$$\begin{aligned}&\sum_{mj=1}^{n_a}P_{ai}C_{aa}(\mathbf{x}_j,\mathbf{x}_{mj})+\sum_{mk=1}^{n_h}Q_{ak}C_{ah}(\mathbf{x}_j,\mathbf{x}_{mk})+\sum_{ml=1}^{n_s}R_{al}C_{as}(\mathbf{x}_j,\mathbf{x}_{ml})\\ &\qquad=C_{aa}(\mathbf{x}_j,\mathbf{x}_0)\\ &\sum_{mj=1}^{n_a}P_{ai}C_{ha}(\mathbf{x}_k,\mathbf{x}_{mj})+\sum_{mk=1}^{n_h}Q_{ak}C_{hh}(\mathbf{x}_k,\mathbf{x}_{mk})+\sum_{ml=1}^{n_s}R_{al}C_{hs}(\mathbf{x}_k,\mathbf{x}_{ml})\\ &\qquad=C_{ha}(\mathbf{x}_k,\mathbf{x}_0)\end{aligned} \tag{8}$$

$$\sum_{mj=1}^{n_a} P_{ai} C_{sa}(\mathbf{x}_l, \mathbf{x}_{mj}) + \sum_{mk=1}^{n_h} Q_{ak} C_{sh}(\mathbf{x}_l, \mathbf{x}_{mk}) + \sum_{ml=1}^{n_s} R_{al} C_{ss}(\mathbf{x}_l, \mathbf{x}_{ml}) = C_{sa}(\mathbf{x}_l, \mathbf{x}_0)$$

where C_{ff}, C_{aa}, C_{hh}, and C_{ss} are the autocovariance functions of f, a, h, and s, respectively, and the others C_{pq} (p, $q = f$, a, h, or s) are cross-covariance functions between p and q.

The cokriging variances associated with these estimates are given by

$$\sum_f = C_{ff}(\mathbf{x}_0, \mathbf{x}_0) - \sum_{i=1}^{n_f} P_{fi} C_{ff}(\mathbf{x}_i, \mathbf{x}_0) - \sum_{k=1}^{n_h} Q_{fk} C_{fh}(\mathbf{x}_k, \mathbf{x}_0) - \sum_{l=1}^{n_s} R_{fl} C_{fs}(\mathbf{x}_l, \mathbf{x}_0)$$
$$\sum_a = C_{aa}(\mathbf{x}_0, \mathbf{x}_0) - \sum_{j=1}^{n_a} P_{aj} C_{aa}(\mathbf{x}_j, \mathbf{x}_0) - \sum_{k=1}^{n_h} Q_{ak} C_{ah}(\mathbf{x}_k, \mathbf{x}_0) - \sum_{l=1}^{n_s} R_{al} C_{as}(\mathbf{x}_l, \mathbf{x}_0) \tag{9}$$

where Σ_f and Σ_a denote the cokriging variance of $\ln K_s$ and α estimates, respectively.

Theoretically, if all the variables are jointly normal, the above approach should produce the conditional mean estimates and conditional variances. Using Monte Carlo simulation, *Yeh* [1989] demonstrated that under one-dimensional flow conditions, h and f are likely to be jointly normal. However, the result was derived from numerical simulations of uniform flow in random porous media, and its validity remains to be tested in the field. To be conservative, we say our estimates are approximate conditional mean fields and variances.

Evaluation of Covariances and Cross Covariances

In order to determine the cokriging coefficients in (7) and (8), autocovariance and cross-covariance functions of the random variables f, a, h, and s must be specified. The autocovariance functions of f and a fields, in general, can be estimated from the field data set. The cross covariance of f, a, h, and s and the autocovariance functions of h and s for unsaturated flow can be obtained either by (1) statistical analysis of the observed data set or results from Monte Carlo simulations, (2) first-order perturbation approximation of the stochastic flow governing equation via spectral-perturbation technique [e.g., *Yeh et al.*, 1985 a, b], or (3) the combination of first-order Taylor series approximation of flow equation and sensitivity analysis [e.g., *Dettinger and Wilson*, 1981; *Hoeksema and Kitanidis*, 1984].

Statistical analysis of the sampled data requires a large number of samples of f, a, h, and s in order to estimate the cross covariance and covariance functions. The estimated functions may, however, not be positive definite, and this can cause numerical problems in solving (7) and (8). Functions derived from Monte Carlo simulations also suffer from the same mathematical difficulties. On the other hand, the covariance and cross-covariance functions derived from the spectral analysis are free from this problem, but they are limited to infinite domains (without the effects of boundaries) as well as stationary random processes. To alleviate the problem associated with the spectral technique, an approach based on the first-order Taylor series approximation of the numerical model of (1) is used to evaluate these covariance functions. Similar to the spectral approach, this numerical approach is, however, limited to small variation in the hydraulic parameters because of the first-order approximation. The development of the numerical approach is given as follows.

If we choose a finite element method to descritize (1), it can be written in a matrix form

$$[\mathbf{G}]\{\boldsymbol{\psi}\} = \{\mathbf{B}\} \tag{10}$$

where $[\mathbf{G}]$ is the coefficient matrix, $\{\mathbf{B}\}$ is the vector associated with boundary conditions, and $\{\boldsymbol{\psi}\}$ is the solution vector. Furthermore, $\{\boldsymbol{\psi}\}$ can be written as

$$\{\boldsymbol{\psi}\} = [\mathbf{G}]^{-1}\{\mathbf{B}\} \tag{11}$$

Assume $\{\mathbf{F}\}$ and $\{\mathbf{A}\}$ are the vectors of the mean values of log-saturated hydraulic conductivity and pore-size distribution parameter, $\{\mathbf{F}\} = E[\{\ln \mathbf{K}_S\}]$ and $\{\mathbf{A}\} = E[\{\ln \boldsymbol{\alpha}\}]$, and $\{\mathbf{H}\}$ is the vector of soil-water pressure evaluated at $\{\mathbf{F}\}$ and $\{\mathbf{A}\}$. Let $\{\mathbf{f}\}$ and $\{\mathbf{a}\}$ be the perturbation vectors of $\{\ln \mathbf{K}_s\}$ and $\{\ln \boldsymbol{\alpha}\}$, and $\{\mathbf{h}\}$ be the deviation of soil-water pressure from $\{\mathbf{H}\}$. Furthermore, if we assume that the magnitudes of perturbation vectors $\{\mathbf{f}\}$ and $\{\mathbf{a}\}$ are small, we may approximate the soil-water pressure head $\{\boldsymbol{\psi}\}$ with a multivariate first-order Taylor series approximation of (11) at $\{\mathbf{F}\}$ and $\{\mathbf{A}\}$:

$$\{\boldsymbol{\psi}\} = \{\mathbf{H}\} + \{\mathbf{h}\} = \mathbf{g}(\{\mathbf{F}\} + \{\mathbf{f}\}, \{\mathbf{A}\} + \{\mathbf{a}\}) \approx \mathbf{g}(\{\mathbf{F}\}, \{\mathbf{A}\}) + \left[\frac{\partial \psi}{\partial \ln K_s}\right]_{(\{\mathbf{F}\},\{\mathbf{A}\})} \{\mathbf{f}\} + \left[\frac{\partial \psi}{\partial \ln a}\right]_{(\{\mathbf{F}\},\{\mathbf{A}\})} \{\mathbf{a}\} \tag{12}$$

where $\mathbf{g}$ represents the matrix representation of (11). After subtracting the expected value of (12) from (12) itself, the first-order approximation of the perturbation of soil-water pressure can be written as

$$\{\mathbf{h}\} \approx \left[\frac{\partial \psi}{\partial \ln K_s}\right]_{(\{\mathbf{F}\},\{\mathbf{A}\})} \{\mathbf{f}\} + \left[\frac{\partial \psi}{\partial \ln a}\right]_{(\{\mathbf{F}\},\{\mathbf{A}\})} \{\mathbf{a}\} = [\mathbf{J}^{(h,f)}]\{\mathbf{f}\} + [\mathbf{J}^{(h,a)}]\{\mathbf{a}\} \tag{13}$$

where matrices $[\mathbf{J}^{(hf)}]$ and $[\mathbf{J}^{(ha)}]$ are the sensitivity matrices of $\{\mathbf{h}\}$ with respect to $\{\mathbf{f}\}$ and $\{\mathbf{a}\}$ evaluated at the mean values $\{\mathbf{F}\}$ and $\{\mathbf{A}\}$, respectively.

Performing some simple statistical operations using (13), the covariance function of $\{\mathbf{h}\}$ and cross-covariance functions between $\{\mathbf{h}\}$ and $\{\mathbf{f}\}$ and $\{\mathbf{a}\}$ can be approximated as

$$[\mathbf{C}_{fh}] \approx [\mathbf{J}^{(hf)}][\mathbf{C}_{ff}]$$
$$[\mathbf{C}_{ah}] \approx [\mathbf{J}^{(ha)}][\mathbf{C}_{aa}] \tag{14}$$
$$[\mathbf{C}_{hh}] \approx [\mathbf{J}^{(hf)}][\mathbf{C}_{ff}][\mathbf{J}^{(hf)}]^T + [\mathbf{J}^{(ha)}][\mathbf{C}_{aa}][\mathbf{J}^{(ha)}]^T$$

where $[\mathbf{J}]^{\mathrm{T}}$ is the transpose of the sensitivity matrix $[\mathbf{J}]$ and $[\mathbf{C}_{ff}]$ and $[\mathbf{C}_{aa}]$ are the specified autocovariances of log-saturated hydraulic conductivity $\ln K_s$ and log pore size distribution coefficient $\ln \alpha$, respectively.

In the same way the sensitivity matrices of effective saturation $\{\boldsymbol{\Theta}\}$ with respect to $\{\ln K_s\}$ and $\{\ln \alpha\}$ are defined as

$$[\mathbf{J}^{(sf)}] = \left[\frac{\partial \Theta}{\partial \ln K_s}\right] \qquad [\mathbf{J}^{(sa)}] = \left[\frac{\partial \Theta}{\partial \ln \alpha}\right] \tag{15}$$

Thus, the approximate cross-covariance functions between $\{\mathbf{f}\}$, $\{\mathbf{a}\}$, and $\{\mathbf{s}\}$ are

$$[\mathbf{C}_{fs}] \approx [\mathbf{J}^{(sf)}][\mathbf{C}_{ff}]$$
$$[\mathbf{C}_{as}] \approx [\mathbf{J}^{(sa)}][\mathbf{C}_{aa}] \tag{16}$$
$$[\mathbf{C}_{ss}] \approx [\mathbf{J}^{(sf)}][\mathbf{C}_{ff}][\mathbf{J}^{(sf)}]^T + [\mathbf{J}^{(sa)}][\mathbf{C}_{aa}][\mathbf{J}^{(sa)}]^T$$

and the cross-covariance function between $\{\mathbf{s}\}$ and $\{\mathbf{h}\}$ can be expressed as

$$[\mathbf{C}_{hs}] \approx [\mathbf{J}^{(sf)}][\mathbf{C}_{ff}][\mathbf{J}^{(hf)}]^T + [\mathbf{J}^{(sa)}][\mathbf{C}_{aa}][\mathbf{J}^{(ha)}]^T \tag{17}$$

Notice that the above cross-covariance and covariance functions related to flow processes (soil-water pressure head h and effective saturation s) may vary with the locations and are not necessarily functions of separation distance only. Such a nonstationary behavior in the covariances is expected since the flow process is nonstationary because of the finite and bounded domain considered in the study.

Adjoint Sensitivity Analysis

To evaluate the sensitivity matrices of $[\mathbf{J}^{(hf)}]$, $[\mathbf{J}^{(ha)}]$, $[\mathbf{J}^{(sf)}]$, and $[\mathbf{J}^{(sa)}]$, the adjoint sensitivity theory is employed. The adjoint state approach has been widely applied to groundwater flow problems [e.g., *Neuman*, 1980; *Sykes et al*., 1985; *Sun and Yeh*, 1992]. Its application to unsaturated flow problems, however, has been limited. Here we followed the approach for saturated flow developed by *Sykes et al*. [1985].

In adjoint sensitivity theory the Richards equation (1) with boundary conditions (2) is defined as the "primary" problem. Consider that the solution domain of the primary problem is discretized into M elements with L nodal points and $\ln K_s$ and $\ln \alpha$ are defined at every element. If ψ is the soil-water pressure at some locations $\mathbf{x}_n$ in the domain ($n = 1, 2, \cdots, N$), the sensitivities matrices ($\mathbf{N} \times \mathbf{M}$) of $\boldsymbol{\psi}$ with respect to $\ln K_s$ and $\ln \alpha$ can be defined as

$$\mathbf{J}^{(hf)}(n, m) = \frac{\partial \psi_n}{\partial(\ln K_s)_m} \qquad \mathbf{J}^{(ha)}(n, m) = \frac{\partial \psi_n}{\partial(\ln \alpha)_m} \tag{18}$$

To evaluate (18), we choose a performance measure:

$$P = \int_\Omega \mathcal{F}(\{\boldsymbol{\beta}\}, \phi)\, d\Omega \tag{19}$$

where Ω is the flow domain bounded by boundary Γ. $\mathcal{F}(\{\boldsymbol{\beta}\}, \phi)$ is a user-chosen function of system state ϕ and system parameters vector $\{\boldsymbol{\beta}\}$. In this study the system state is the total hydraulic head $\phi = \psi + x_2$, and system parameters $\{\boldsymbol{\beta}\}$ are $\ln K_s$, $\ln \alpha$, prescribed head boundary condition ϕ^*, and prescribed flux boundary conditions q^*.

The sensitivity of the performance measure P to any specific parameter β_k is defined as $dP/d\beta_k$ and can be expressed as

$$\frac{dP}{d\beta_k} = \int_\Omega \left[\frac{\partial \mathcal{F}(\{\boldsymbol{\beta}\}, \phi)}{\partial \beta_k} + \frac{\partial \mathcal{F}(\{\boldsymbol{\beta}\}, \phi)}{\partial \phi} \gamma \right] d\Omega \tag{20}$$

where $\gamma = d\phi/d\beta_k$ is the sensitivity of the total head to parameter β_k and is called "state sensitivity." This state sensitivity can be evaluated by solving a new differential equation (sensitivity equation) derived by differentiating (1) with respect to a specific parameter β_k:

$$\frac{\partial}{\partial x_i}\left(\frac{\partial K}{\partial \beta_k}\frac{\partial \phi}{\partial x_i} + K \frac{\partial \gamma}{\partial x_i}\right) = 0 \qquad i = 1, 2 \tag{21}$$

The boundary conditions associated with (21) are

$$\gamma = \frac{\partial \phi^*}{\partial \beta_k} \qquad \text{on } \Gamma_1$$
$$\frac{\partial q^*}{\partial \beta_k} n_i + \frac{\partial q^*}{\partial h} \gamma n_i = \frac{\partial q^*}{\partial \beta_k} \qquad \text{on } \Gamma_2 \tag{22}$$

Sensitivity equation (21) has a similar structure to its original equation (1). With boundary conditions (22), (21) can be solved numerically to obtain the state sensitivity γ. For each specific parameter β_k, sensitivity equation (21) has to be solved once to evaluate the sensitivity of performance measure P to the parameter β_k. If the system includes a large number of parameters β_k, as in our analysis, this approach is time-consuming [*Kabala and Milly*, 1990]. Alternatively, we can avoid the direct evaluation of state sensitivity by formulating adjoint equations of the partial differential equations for γ.

Multiplying (21) by an arbitrary differentiable function λ and integrating over the flow domain Ω gives,

$$\int_\Omega \left[\lambda \frac{\partial}{\partial x_i}\left(K \frac{\partial \gamma}{\partial x_i}\right) + \lambda \frac{\partial}{\partial x_i}\left(\frac{\partial K}{\partial \beta_k}\frac{\partial \phi}{\partial x_i}\right)\right] d\Omega = 0 \tag{23}$$

Applying Green's first identity to (23) then adding the resultant to the sensitivity of performance measure (20) yields,

$$\frac{dP}{d\beta_k} = \int_\Omega \left\{ \frac{\partial \mathcal{F}(\{\boldsymbol{\beta}\}, \phi)}{\partial \beta_k} + \gamma \left[\frac{\partial \mathcal{F}(\{\boldsymbol{\beta}\}, \phi)}{\partial \phi} + \frac{\partial}{\partial x_i \left(K \dfrac{\partial \lambda}{\partial x_i}\right)} \right] - \frac{\partial \lambda}{\partial x_i}\frac{\partial K}{\partial \beta_k}\frac{\partial \phi}{\partial x_i} \right\} d\Omega + \int_\Gamma \left(\gamma K \frac{\partial \lambda}{\partial x_i} n_i + \lambda \frac{\partial q_1}{\partial \beta_k}\right) d\Gamma \tag{24}$$

To eliminate the unknown state sensitivities γ in (24), an arbitrary function λ is chosen to satisfy the following equation and boundary conditions, known as the adjoint problem:

$$\frac{\partial \mathcal{F}(\{\boldsymbol{\beta}\}, \phi)}{\partial \phi} + \frac{\partial}{\partial x_i}\left(K \frac{\partial \lambda}{\partial x_i}\right) = 0 \tag{25}$$

associated with boundary conditions,

$$\lambda = 0 \qquad \text{on } \Gamma_1$$
$$K \frac{\partial \lambda}{\partial x_i} n_i = 0 \qquad \text{on } \Gamma_2 \tag{26}$$

To evaluate the sensitivity matrices of total hydraulic head with respect to $\ln K_s$ and $\ln \alpha$, we define $\beta_k = \ln K_s$ and $\beta_k = \ln \alpha$, respectively, and choose the user-defined function of (19) as

$$\mathcal{F}(\{\boldsymbol{\beta}\}, \phi) = \phi \delta(\mathbf{x} - \mathbf{x}_p) \tag{27}$$

Therefore the adjoint sensitivity equation (25) becomes

$$\frac{\partial}{\partial x_i}\left(K \frac{\partial \lambda}{\partial x_i}\right) = -\delta(\mathbf{x} - \mathbf{x}_p) \tag{28}$$

where $\delta(\mathbf{x} - \mathbf{x}_p)$ is the Dirac delta function, and $\mathbf{x}_p$ is the location where the sensitivity of head to changes of parameters is to be calculated. As (28) is similar to primary problem (1) with the exception that K is known and independent of λ and the right-hand side is the Dirac delta function instead of zero, (28) is linear and can be solved numerically just like a saturated flow problem.

With the adjoint function (28) associated with boundary conditions (26) the sensitivity performance measure (20) can be determined by evaluating

$$\frac{\partial \psi_p}{\partial \beta_k} = \int_\Omega \left[-\frac{\partial \lambda}{\partial x_i} \frac{\partial K}{\partial \beta_k} \frac{\partial \phi}{\partial x_i} \right] d\Omega \tag{29}$$

Notice that $dP/d\beta_k = d\phi(\mathbf{x}_p)/d\beta_k = d\psi(\mathbf{x}_p)/d\beta_k$ because $P = \phi(\mathbf{x}_p) = \psi_I(\mathbf{x}_p) + x_2$. Compared with directly solving the state sensitivity equation of (21), the major advantage of adjoint sensitivity analysis is that for different β_k the adjoint equation needs to be solved only once for a specific user-chosen function $\mathcal{F}$.

If the system parameter β_k denotes the log-saturated hydraulic conductivity in the element k, or $(\ln K_s)_k$, and the exponential model (3) is used, then

$$J^{(hf)}(p, k) = \frac{\partial \psi_p}{\partial (\ln K_s)_k} = -\sum_{l=1}^{M} u_1 \int_{\Omega_l} \frac{\partial \lambda}{\partial x_i} \frac{\partial \phi}{\partial x_i} d\Omega \tag{30}$$

where l is the element index, M is the total number of elements, and Ω_l is the domain of element l. In addition,

$$u_l = \frac{\partial K_l}{\partial (\ln K_s)_k} = K_l \left[\delta_{kl} + \alpha_l \frac{\partial \psi_l}{\partial (\ln K_s)_k} \right] \tag{31}$$

where K_l and α_l are the unsaturated conductivity and pore size distribution coefficient, respectively, of element l. The variable δ is the Kronecker delta ($\delta_{kl} = 1$ for $k = l$ and 0 otherwise).

If we define the integral in (30) as

$$S(p, l) = -\int_{\Omega_l} \frac{\partial \lambda}{\partial x_i} \frac{\partial \phi}{\partial x_i} d\Omega \tag{32}$$

in which the adjoint function λ is associated with the pressure head ψ_p located at $\mathbf{x}_p$, $S(p, l)$ can be evaluated numerically with the known λ and ϕ distributions in the flow domain. Therefore (32) can be rewritten as

$$\sum_{l=1}^{M} [\delta_{pl} - K_l \alpha_l S(p, l)] J^{(hf)}(l, k) = -K_k S(p, k) \tag{33}$$

$$p = 1, 2, \cdots, M$$

The sensitivity of soil-water pressure ψ_l with respect to $\ln K_s$ can then be obtained by solving matrix equation (33) which contains M unknowns $J(p, k)$, ($p = 1, 2, \cdots, M$, and k is fixed) with M equations. Notice that in (33) the matrix is independent of the element index k. Hence the matrix has to be evaluated only once, and the solution can be used directly to determine $J(p, k)$ for other elements.

Similarly, if the system parameter β_k is defined as a log pore size distribution coefficient on element k, that is, $\beta_k = (\ln \alpha)_k$, the matrix equation of the sensitivities of soil-water pressures in all elements with respect to $\ln \alpha$ of one element k, $J^{(ha)}(p, k) = \partial \psi_i / \partial (\ln \alpha)_k$ can be obtained as

$$\sum_{l=1}^{M} [\delta_{pl} - K_l \alpha_l S(p, l)] J^{(ha)}(l, k) = -K_k \alpha_k \psi_k S(p, k) \tag{34}$$

$$p = 1, 2, \cdots, M$$

After sensitivity matrices of soil-water pressure with respect to $\ln K_s$ and $\ln \alpha$ are derived, sensitivity matrices of effective saturation Θ with respect to $\ln K_s$ and $\ln \alpha$ can be evaluated easily as follows.

Since very little information about the spatial statistics of τ is available, the degree of saturation expressed by (4) is thus simplified by taking τ as zero [*Russo*, 1988]. That is,

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = e^{0.5\alpha\psi}(1 - 0.5\alpha\psi) \tag{35}$$

Then, taking derivatives of Θ with respect to $\ln K_s$ and $\ln \alpha$ yields

$$\begin{aligned} \frac{\partial \Theta_i}{\partial (\ln K_s)_j} &= -0.25\alpha_i^2 \psi_i e^{0.5\alpha_i\psi_i} \frac{\partial \psi_i}{\partial (\ln K_s)_j} \\ \frac{\partial \Theta_i}{\partial (\ln \alpha)_j} &= -0.25\alpha_i^2 \psi_i e^{0.5\alpha_i\psi_i} \left[\psi_i \delta_{ij} + \frac{\partial \psi_i}{\partial (\ln \alpha)_j} \right] \end{aligned} \tag{36}$$

Once the sensitivities $\partial \psi_i / \partial (\ln K_s)_j$ and $\partial \psi_i / \partial (\ln \alpha)_j$ are evaluated, the sensitivities $\partial \Theta_i / \partial (\ln K_s)_j$ and $\partial \Theta_i / \partial (\ln \alpha)_j$ can be calculated using (36). Subsequently, all of the sensitivity matrices of $[\mathbf{J}^{(\mathrm{hf})}]$, $[\mathbf{J}^{(\mathrm{ha})}]$, $[\mathbf{J}^{(\mathrm{sf})}]$, and $[\mathbf{J}^{(\mathrm{sa})}]$ can be obtained.

Numerical Examples

As mentioned previously, detailed characterization of a vadose zone is a difficult and expensive task. Consequently, few field experiments have been conducted in the past to provide sufficient data sets for testing any inverse models, and we have to rely on numerical experiments to test our geostatistical inverse approach. The numerical experiments involved steady state flows in a 7 m × 7 m vertical plane of a hypothetical vadose zone. The left and right boundaries of the flow domain were defined as impermeable, and the lower boundary was considered as a prescribed head boundary, while the upper boundary condition varied for different flow scenarios. The flow domain is discretized uniformly into 35 × 35 finite element with $dx = dy = 20$ cm. Each element is assigned a saturated hydraulic conductivity value and a pore size distribution coefficient value created from a random field generator [*Gutjahr*, 1989] with a modified form of the Whittle spectrum (spectrum A, anisotropic case [*Mizell et al.*, 1982]). The variances of $\ln K_s$ and $\ln \alpha$ are taken as 1.0 and 0.1, respectively, while the mean value of $\ln K_s$ is given as -3.0 and the mean of $\ln \alpha$ is 0.0. The correlation scales for both $\ln K_s$ and $\ln \alpha$ are set to be 100 cm and 300 cm in the vertical and horizontal directions, respectively. The synthesized $\ln K_s$ and $\ln \alpha$ fields are shown in the top row of Figure 2. Once the hypothetical vadose zone is generated, a finite element model [*Yeh et al.*, 1993] is used to solve the primary flow problem (1) to obtain the pressure head and saturation fields. These $\ln K_s$, $\ln \alpha$, ψ, and Θ fields are then regarded as the real-world analogues (true fields) where measurements of these parameters are taken. Sixteen $\ln K_s$ and $\ln \alpha$ values ($n_f = n_a = 16$) were sampled at a 4 × 4 uniform grid over the entire domain as our primary information. The secondary information, pressure head values, was then taken from a 10 × 10 uniform grid, resulting in a total

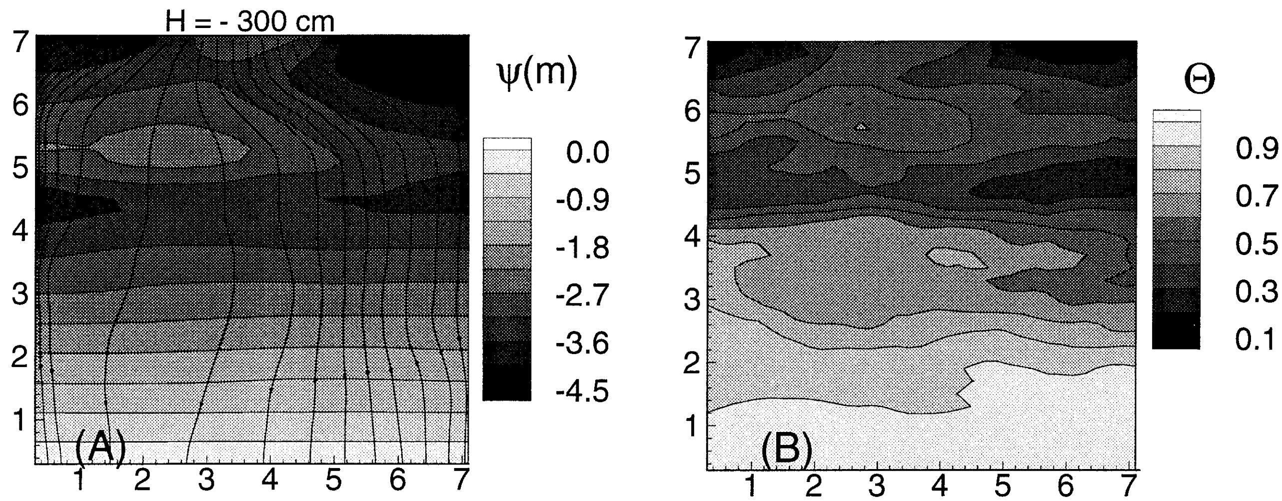

Figure 1. Distributions of (a) soil-water pressure head in meters, ψ, and the streamline, and (b) degree of saturation, Θ, in the hypothetical vadose zone.

of 100 pressure head measurements ($n_h = 100$). Similarly, a total of 81 sampled Θ values ($n_s = 81$) were obtained from a 9×9 uniform sampling grid.

Three flow cases, case 1, nonuniform flow A, case 2, nonuniform flow B, and case 3, uniform flow, associated with different upper boundary conditions, are considered here to investigate the usefulness of the primary and secondary information on the estimation of $\ln K_s$ and $\ln \alpha$ fields. In case 1, the lower boundary is set to be the water table and the central ten nodes of the upper boundary are constant heads (-100, -300, and -500 cm), while the remaining parts are no-flux boundaries. The true soil-water pressure head, flow, and degree of saturation fields for this case with upper boundary of -300 cm pressure head are shown in Figures 1a and 1b. Since the mean soil-water pressure head varies, the mean gradient changes with location. As a result, the h and s fields are nonstationary.

In case 2, the boundary conditions are the same as case 1 except that the entire upper boundary is set to be a prescribed constant head. The mean soil-water pressure head field varies with depth. It becomes less negative as it approaches the water table, and the h and s fields are nonstationary. In this case, three different prescribed head values (-100, -300, and -500 cm) for the upper boundary condition are also considered.

The upper boundary conditions in case 3 were set to the same prescribed head values as the lower boundary conditions. The same as the previous cases, three different prescribed head values (-100, -300, and -500 cm) were used. The mean flow in this case is uniform in most of the domain with the hydraulic gradient of 1 (unit gradient case) except near the left- and right-hand-side boundaries (no flow). Under this condition the h and s fields away from the boundaries are essentially stationary.

For the above three cases, four different geostatistical estimation approaches are employed to estimate $\ln K_s$ and $\ln \alpha$ fields. Approach 1 uses simple kriging with the primary information (the $\ln K_s$ and $\ln \alpha$ measurements) only. In approach 2 our cokriging technique is employed using both the soil-water pressure information and the primary information. In contrast to approach 2, approach 3 uses the effective saturation information and the primary information. Finally, approach 4 utilizes all the information (measurements of $\ln K_s$, $\ln \alpha$, soil-water pressure, and effective saturation) to conduct cokriging.

The performance of each approach under different flow conditions and wetness of the flow field is assessed by two quantitative measures. The first is the mean square error (MSE),

$$\mathrm{MSE} = \frac{1}{N} \sum_{i=1}^{N} (y_{oi} - y_{ei})^2 \tag{37}$$

where y_{oi} and y_{ei} are the observed and estimated parameter values at the ith location, respectively, and N is the total number of elements for f. The second is the (co)kriged variance (9), which evaluates the ability of each approach in reducing the prediction variance in the ensemble sense.

Results and Discussion

Figure 2 illustrates the estimated $\ln K_s$ and $\ln \alpha$ fields of case 1 by the above mentioned four different approaches. Rectangles in Figure 2 represent the sample locations of $\ln K_s$ and $\ln \alpha$, sample locations for h and s are denoted by circles and squares, respectively. As expected, the kriged $\ln K_s$ and $\ln \alpha$ fields based on the primary information only are much smoother than the true fields, while the fields produced by the approaches using both primary and secondary information reveal some details of the heterogeneity of the real-world analog.

Tables 1, 2, and 3 tabulate the quantitative assessment of the performance of these four approaches for all the cases. The first rows of these tables list the values of the mean square errors and estimation variances for $\ln K_s$ and $\ln \alpha$ estimates based on kriging (approach 1). Notice that the result of this approach does not vary with cases. The percentage of the improvement due to the use of the geostatistical inverse technique along with different secondary information is listed in the other rows. This percentage represents the difference between the result of approach 1 and the others (approaches 2, 3, and 4) normalized by the result of approach 1. A positive value implies improvement and a negative value denotes deterioration. These tables show that the geostatistical inverse approach consistently yields better estimates than kriging. The mean square errors of the ln K_s and ln α fields by the inverse model are always smaller than those of kriging. Similarly, the estimation variances of the ln K_s and ln α fields from the inverse approach are less than those of kriging.

In addition, approach 2 using h measurements improves the estimation of ln K_s in all cases, but the improvement decreases as the soil becomes dry. The impact of h measurements on the estimation of ln α is smaller than that on the ln K_s under wet conditions; it becomes greater as the soil becomes less saturated. Using the information about the effective saturation, s, approach 3 dramatically enhances the estimation of ln α, especially in the relatively dry soils. Under wet conditions (e.g., $H = -100$ cm) the improvement is not significant, because some areas of the soil profile were saturated and the effective saturation no longer depends on the value of ln α. The effectiveness of approach 3 on the estimation of ln K_s drops rapidly as the value of H becomes more negative. For all the cases, approach 4 using both the primary (f and a) and secondary (h and s) information yields much better estimates than the others. In general, the flow field (uniform or nonuniform) does not significantly affect the geostatistical inverse approach.

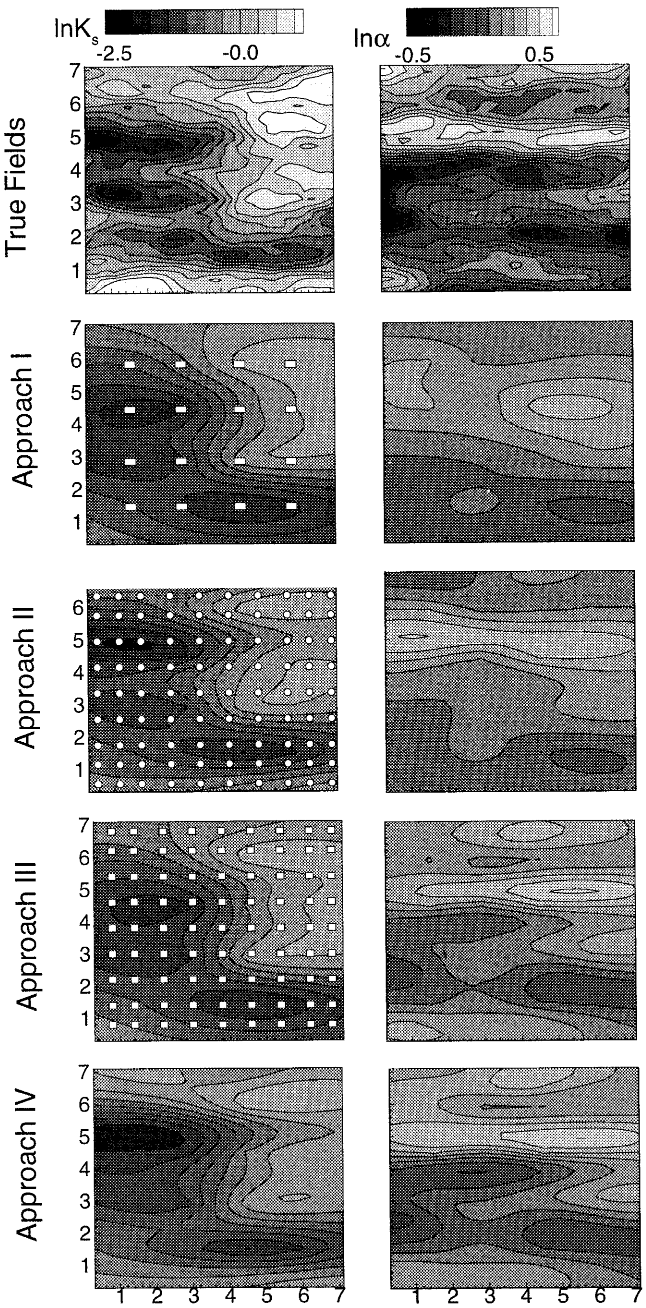

Figure 2. Comparison of true ln K_s and ln α fields with those derived from the four different approaches.

Table 1. Comparison of Results of the Four Approaches for Case 1

Head, cm	Approach	MSE ln K_s	MSE ln α	Σ ln K_s	Σ ln α
	1 (f, a)	0.3570	0.0454	0.4063	0.0406
$H = -100$	2 (f, a, h)	45%	35%	41%	10%
	3 (f, a, s)	36%	46%	15%	36%
	4 (f, a, h, s)	65%	71%	50%	47%
$H = -300$	2 (f, a, h)	19%	46%	31%	18%
	3 (f, a, s)	4%	72%	3%	46%
	4 (f, a, h, s)	34%	83%	47%	50%
$H = -500$	2 (f, a, h)	10%	41%	26%	21%
	3 (f, a, s)	1%	78%	0.5%	49%
	4 (f, a, h, s)	12%	80%	45%	50%

H is the constant soil-water pressure at the central part of the upper boundary. MSE, mean standard error.

The above numerical results are directly related to the cross correlation between the primary and secondary information. To gain some insights into the behavior of the cross correlation, analytical expressions of the cross-correlation functions between f and h, and a and h, are derived. Since two-dimensional analytical results are difficult to obtain, the analysis assumes that the flow is one-dimensional and under steady state and unit-mean-gradient conditions, and the spectral/perturbation approach [*Yeh et al.*, 1985a, b] is used. The analytical expression for the cross-correlation function between f and h is

$$\rho_{fh}(\xi) = \frac{C_{fh}(\xi)}{[C_{ff}(0)C_{hh}(0)]^{1/2}}$$

$$= \frac{\sigma_f}{\sqrt{(\sigma_f^2 + \sigma_a^2 H^2)}} e^{(-\xi/\lambda)} \left[\frac{A\lambda}{(A\lambda + 1)} - \frac{\xi}{\lambda} \right] \qquad (38)$$

for $\xi > 0$. When $\xi < 0$,

Table 2. Comparisons of Results of the Four Approaches for Case 2

Head, cm	Approach	MSE ln K_s	MSE ln α	Σ ln K_s	Σ ln α
	1 (f, a)	0.3570	0.0454	0.4063	0.0406
$H = -100$	2 (f, a, h)	55%	17%	48%	3%
	3 (f, a, s)	62%	28%	30%	23%
	4 (f, a, h, s)	71%	33%	52%	42%
$H = -300$	2 (f, a, h)	11%	53%	34%	15%
	3 (f, a, s)	9%	73%	5%	45%
	4 (f, a, h, s)	49%	85%	49%	50%
$H = -500$	2 (f, a, h)	5%	40%	27%	22%
	3 (f, a, s)	1%	78%	1%	48%
	4 (f, a, h, s)	22%	83%	47%	50%

Table 3. Comparisons of Results of the Four Approaches for Case 3

Head, cm	Approach	MSE $\ln K_s$	MSE $\ln \alpha$	Σ $\ln K_s$	Σ $\ln \alpha$
	1 (f, a)	0.3570	0.0454	0.4063	0.0406
$H = -100$	2 (f, a, h)	57%	10%	46%	4%
	3 (f, a, s)	61%	30%	30%	26%
	4 (f, a, h, s)	77%	41%	52%	43%
$H = -300$	2 (f, a, h)	6%	50%	26%	23%
	3 (f, a, s)	34%	74%	10%	41%
	4 (f, a, h, s)	62%	85%	47%	50%
$H = -500$	2 (f, a, h)	−17%	53%	14%	35%
	3 (f, a, s)	19%	74%	4%	45%
	4 (f, a, h, s)	35%	78%	43%	52%

$$\rho_{fh}(\xi) = \frac{\sigma_f}{\sqrt{(\sigma_f^2 + \sigma_a^2 H^2)}} \left\{ \left[\frac{A\lambda(A\lambda + 1)}{(A\lambda - 1)^2} - \frac{|\xi|(A\lambda + 1)}{\lambda(A\lambda - 1)} \right] \cdot e^{(-|\xi|/\lambda)} - \frac{4A^2\lambda^2}{(A\lambda - 1)^2(A\lambda + 1)} e^{(-A|\xi|)} \right\} \tag{39}$$

Similarly, the cross-correlation function between a and h can be derived as

$$\rho_{ah}(\xi) = \frac{C_{ah}(\xi)}{[C_{aa}(0)C_{hh}(0)]^{1/2}} = \frac{-\sigma_a H}{\sqrt{(\sigma_f^2 + \sigma_a^2 H^2)}} e^{(-\xi/\lambda)} \left[\frac{A\lambda}{(A\lambda + 1)} - \frac{\xi}{\lambda} \right] \tag{40}$$

if $\xi > 0$, and

$$\rho_{ah}(\xi) = \frac{-\sigma_a H}{\sqrt{(\sigma_f^2 + \sigma_a^2 H^2)}} \left\{ \left[\frac{A\lambda(A\lambda + 1)}{(A\lambda - 1)^2} - \frac{|\xi|(A\lambda + 1)}{\lambda(A\lambda - 1)} \right] \cdot e^{(-|\xi|/\lambda)} - \frac{4A^2\lambda^2}{(A\lambda - 1)^2(A\lambda + 1)} e^{(-A|\xi|)} \right\} \tag{41}$$

if $\xi < 0$, where ξ is the separation distance (lag), λ is the correlation scale, and σ_f and σ_a are the standard deviation of $\ln K_s$ and $\ln \alpha$, respectively.

It is interesting that under unsaturated conditions the absolute value of ρ_{fh} at any given separation distance decreases as H becomes more negative ((38) and (39)), implying that the drier the soil is the smaller the correlation between f and h is. Subsequently, measurements of h do not improve the estimate of $\ln K_s$ under dry conditions. On the contrary, the absolute value of ρ_{ah} increases as the soil becomes less saturated ((40 and (41)); measurements of h improve the estimate of $\ln \alpha$. As H becomes less negative (approaching zero) or the soil is near saturation, the cross correlation between f and h increases, while the value of ρ_{ah} drops. As a result, measurements of h improve the estimate of $\ln K_s$ but not $\ln \alpha$. When the soil is fully saturated (H and $A = 0$), the behavior of ρ_{fh} is then similar to the two-dimensional result by *Mizell et al.* [1982], which is independent of the mean pressure head, and ρ_{ah} becomes zero.

Formulas similar to (38)–(41) and (39) can also be derived for ρ_{fs} and ρ_{as} to explain the results of approach 3. However, they are far more complex and will not be presented in this paper. Plots of cross-correlation functions, ρ_{ah}, ρ_{fh}, ρ_{fs}, in x_1 and x_2 directions are shown in Figure 3 for the two-dimensional uniform flow case with $H = -100$ cm (solid curve) and -500 cm (dashed curve). In general, the cross-correlation value is higher in the direction of flow (x_2) than in the direction normal to the flow (x_1). It should be pointed out that the errors associated with the first-order approximation of these cross-covariance functions become large when the head perturbation grows as soil becomes less saturated [*Yeh*, 1989].

The geostatistical inverse model has its limitations. It may suffer numerical instability problems similar to those in the classical inverse models for saturated flow [see *Yeh*, 1986]. *Dietrich and Newsam* [1989] pointed out that as the amount of available data increases and the discretization of the system is refined, both a numerically ill-conditioned parameter estimation problem and ill-conditioned cokriging equation may occur; the cokriged transmissivity field may contain some anomalies. To avoid this problem, addition of an error term to the cokriging equation is suggested for stabilizing its numerical solution. They showed that an addition of such an error term may result in the loss of information. In our analysis the amount of primary and secondary information (16(2) + 100 + 81 = 213) is relatively small compared to the total number of parameters (1225 − 16(2) = 1193) to be estimated. The conditional number of the cokriging matrices seems large, but no anomalies were observed in the estimated $\ln K_s$ and $\ln \alpha$ fields for all the cases examined. However, the instability problem may occur as the amount of information increases.

As mentioned previously, our geostatistical inverse approach is a linear predictor. Under fully saturated conditions the linear assumption is valid as long as the variability of the primary variable is small [see *Yeh et al.*, 1996]. The validity of the assumption may be further restricted in the case of variably saturated flow because of the additional nonlinearity in the unsaturated hydraulic conductivity and water release curves. Theoretically, it is difficult to quantify the error associated with this assumption. It is, however, our conjecture that the linear assumption merely reduces the effectiveness of the secondary information. If the nonlinearity can be incorporated into our estimation technique, more detailed spatial distributions of $\ln K_s$ and $\ln \alpha$ fields will be revealed. Nevertheless, for depicting the general spatial patterns of $\ln K_s$ and $\ln \alpha$ fields, such a linear predictor can serve as a useful and practical tool, as demonstrated in our numerical examples.

While results of the numerical experiments appear interesting, application of this geostatistical inverse approach to field

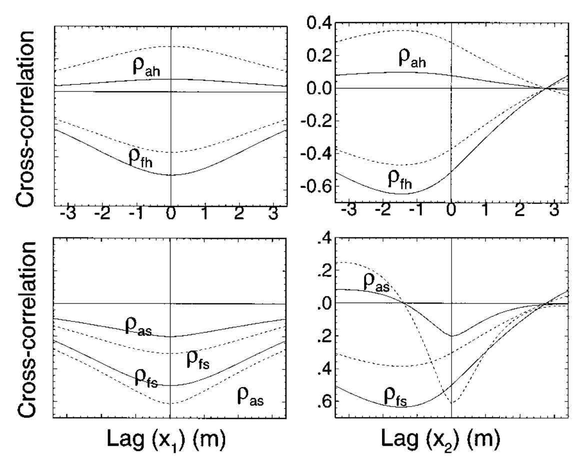

Figure 3. Behaviors of cross-correlation functions in case 3.

situations remains to be explored. Although many complications in the field problem are expected, the principle of the approach is not restricted to the simplified assumptions used in the analysis. For example, cokriging has been applied to transient flow problems in fully saturated aquifers [*Sun and Yeh*, 1992]. Application of our geostatistical inverse method to transient flow problems in the vadose zone requires the consideration of the Richards equation for transient flow as the primary problem in the sensitivity analysis. While formulation of the sensitivity matrix is technically feasible, the actual numerical computation is however beyond our resources at this moment [*Li and Yeh*, 1995]. On the other hand, steady state flow in the vadose zone exists in many practical field problems (such as flow under tailings ponds and irrigated fields). In fact, using controlled irrigation schemes, soil scientists frequently create steady state flow situations in the field to measure hydraulic properties of soils and to investigate transport of solutes [e.g., *Greenholtz et al*., 1988; *Butters et al*., 1989]. Therefore steady state flow is not an oversimplified assumption.

Errors in the measurement of the primary and secondary information are expected in the field problems. Differences in the sample volume of various sampling devices (e.g., tensiometers and neutron probes) also may be considered as part of the error in the measurement. In our approach, variance terms representing the error in the measurement of $\ln K_s$, $\ln \alpha$, ψ, and Θ can be added to the covariances (C_{ff}, C_{aa}, C_{hh}, and C_{ss}) in (7) and (8). Effects of the terms on the estimation have been discussed by *Dietrich and Newsam* [1989] for flow through fully saturated aquifers. Large errors in the measurements will result in the loss of the information and reduce the effectiveness of the geostatistical inverse method. This is also true for any other techniques. In the geostatistical inverse method, evaluation of the covariance functions of f and a may require a sufficient number of measurements, and it will be affected by errors in the measurements [see *Russo and Jury*, 1987a, b]. The maximum likelihood approach proposed by *Kitanidis and Vomvoris* [1983] can be incorporated in our approach to alleviate this problem.

On the basis of the analysis of field data by *Russo and Bouton* [1992] our analysis assumes that f and a are uncorrelated, although the α in their analysis is not equivalent to the one used in this paper. The uncorrelated case represents the worst scenario. A cross correlation between f and a will improve our estimates even if the knowledge about the parameterized model of this cross correlation is incomplete. If this model is perfectly known a priori, measurements of f will greatly improve the estimates of a and vice versa. Subsequently, if ψ measurements improve the estimates of f, it also will improve our estimate of a. By the same token, if Θ measurements improve the estimates of a, it also will improve our estimate of f.

Other models [e.g., *van Genuchten*, 1980; *Brook and Corey*, 1964] for the unsaturated hydraulic properties also can be implemented into our geostatistical approach without difficulties. However, the computational burden will increase significantly and is beyond our capacity at this moment. Rapid advances in computational tools may alleviate this difficulty in the near future but uncertainty about the representativeness of these models for field soils over the full range of saturations remains.

Last, we want to emphasize that our predictive ability of natural processes in a field will always be limited to their "large scale" behaviors, even if the field is extensively characterized. Errors in our conceptual and numerical models and inherent uncertainties in our input parameters restrict our predictive ability. For example, *Yeh et al*. [1995b] used three different mathematic models to interpret 305 slug tests in a 5 m × 5 m field site and obtained three distinctly different sets of hydraulic conductivity values. Nevertheless, all three data sets depicted similar patterns of hydraulic heterogeneity at the field site and in turn produced similar tracer plumes that closely resemble the large scale behaviors of the observed one. Subsequently, *Yeh et al*. [1995b] concluded that delineation of "important" heterogeneities is crucial, and exact characterization of heterogeneities at small scales is superfluous since our measurements always involve some uncertainties that cannot be quantified. With these facts in mind the geostatistical inverse method presented in this paper (although it is our initial attempt) may be considered a useful and cost-effective site characterization tool, since it can delineate the general patterns of the hydraulic heterogeneity in the vadose zone.

Conclusions

On the basis of the results of our studies it appears that the geostatistical inverse approach using both the primary and secondary information is a promising tool for delineating spatial distribution of unsaturated hydraulic heterogeneities. The estimates from the inverse approach are better than those derived from kriging on the basis of primary information only. Furthermore, our results indicate that the degree of improvement on the estimates using either h or s will depend upon the wetness of the soil. This characteristic is different from that of the geostatistical inverse problem in the saturated aquifer. Finally, the usefulness of this approach under field conditions remains to be investigated. Carefully designed field experiments are needed.

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