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An iterative geostatistical inverse method for steady flow in the vadose zone

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Abstract. An iterative geostatistical inverse approach is developed to estimate conditional effective unsaturated hydraulic conductivity parameters, soil-water pressure head, and degree of saturation in heterogeneous vadose zones. This approach is similar to the classical cokriging technique, and it uses a linear estimator that depends on covariances and cross covariances of unsaturated hydraulic parameters, soil-water pressure head, and degree of saturation. The linear estimator is, however, improved successively by solving the governing flow equation and by updating the residual covariance and cross-covariance functions in an iterative manner. As a result, the nonlinear relationship between unsaturated hydraulic conductivity parameters and head is incorporated in the estimation and the estimated fields are approximate conditional means. The ability of the iterative approach is demonstrated through some numerical examples.

Introduction

Predicting water and solute movements in the vadose zone at a reasonable degree of resolution requires a large number of measurements of the unsaturated hydraulic conductivity and other hydraulic properties. Hydraulic conductivity of unsaturated porous media is a nonlinear function of soil-water pressure head or moisture content. Because of the dependence of hydraulic conductivity on soil-water pressure and moisture content, measurements of the unsaturated hydraulic conductivity are difficult, time-consuming, and costly tasks. Subsequently, characterization of the vadose zone using direct measurements of the hydraulic conductivity at a large number of locations in the vadose zone has rarely been conducted. On the other hand, information about soil-water pressure head and water content can be collected with relative ease in most shallow and unconsolidated vadose zones, using tensiometers, neutron probes, time domain reflectrometers, and electrical resistivity tomography. Poorly sorted alluvial deposits, conglomerates, and solid rock masses comprising the vadose zone in the western region of United States often prohibit the use of pressure measurement devices. In this case, water content may be the only information that can be collected in large quantities. For these reasons, taking advantage of the abundance of the information about both soil-water pressure and water content to improve our estimates of unsaturated hydraulic properties in the field seems logical. This parameter estimation task thus becomes the so-called inverse problem.

Inverse problems have been a major focus of groundwater hydrology during the past few decades. Many mathematical models have been developed to estimate transmissivity of aquifers with given scattered hydraulic head ϕ and transmissivity measurements (see *Yeh* [1986] for a detailed review). One popular method is the minimum-output-error based approach (e.g., *Yeh and Tauxe*, 1971; *Gavalas et al*., 1976; *Willis and Yeh*, 1987; *Cooley*, 1982; *Carrera and Neuman*, 1986a, b]. Application of this methodology to variably saturated flow in the vadose zone is, however, limited because of the complex nonlinear nature of the governing flow equation (the Richards equation). *Kool and Parker* [1988] and *Russo et al*. [1991] applied this minimum-output-error based approach to one-dimensional unsaturated flow situations, with the goal of estimating parameter values for unsaturated porous media in the laboratory soil column.

While the minimum-output-error based approach faces many inherent numerical difficulties, the geostatistical inverse technique (cokriging) has received increasing attention in recent years. It relies on classical linear predictor theory that takes advantage of spatial correlation structures of pressure head and conductivity and cross correlations between the head and conductivity of porous media. This approach has been widely used to estimate transmissivity, head, velocity, and concentration of pollutants in highly heterogeneous 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*., 1995, 1996]. In the vadose zone it has been applied to estimate water content distribution, based on some measurements of water content, soil-water pressure head, soil surface temperature, and soil texture [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).

Recently, *Harter and Yeh* [1996b] showed, using cokriging and a numerical model, that a large amount of soil-water pressure head measurements can greatly improve the prediction of movement of solutes in the vadose zone. *Yeh and Zhang* [1996] developed a geostatistical inverse (or cokriging) technique for identifying unsaturated hydraulic parameters in heterogeneous vadose zones under steady state nonuniform flow conditions. They found that unsaturated hydraulic parameters of heterogeneous vadose zones can be reasonably identified if a large amount of information on the soil-water pressure and degrees of saturation are used. Their study also revealed that the cross correlation between flow process and hydraulic pa-

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rameters varies with the mean soil-water pressure. As a result, information on soil-water pressure under wet conditions improves the estimate of saturated hydraulic conductivity. On the other hand, information about degree of saturation enhances the estimate of the pore-size distribution parameter in the Gardner-Russo model [*Russo*, 1988].

While results of cokriging appear interesting and promising, limitations of cokriging exist. In this study the limitations are discussed and an iterative geostatistical approach attempting to alleviate these limitations is presented. Using several numerical examples, advantages of the iterative approach over cokriging are illustrated. We hope our preliminary attempt will stimulate more research on this challenging problem of identification of unsaturated hydraulic parameters in the heterogeneous vadose zone.

Statements of Problems

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

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

with specified boundary conditions on Γ_1:

$$\begin{aligned}\psi &= \psi_0 \\ q_i \cdot n_i &= q_0\end{aligned} \tag{2}$$

where x_1 and x_2 are horizontal and vertical coordinates (positive upward), respectively. In (1), ψ is the soil-water pressure head and is positive for saturated flow and negative for unsaturated flow; ψ_0 is the prescribed head on boundary Γ_1, and q_0 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. The Gardner-Russo model [*Russo*, 1988] is used in this study 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:

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

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. The parameter m is a soil parameter that accounts for the tortuosity of the flow path and the correlation between pores. For simplicity, m is set to zero in our study.

In general, solutions to inverse problems of flow through porous media are nonunique. It is a well-known fact that uniquely identifying the spatial distribution of transmissivity in an aquifer under steady state flow conditions is impossible unless all hydraulic heads are known and boundary fluxes are specified. For cases with given scattered hydraulic head ϕ and conductivity or transmissivity measurements, a logical inverse approach should rely on the conditional stochastic concept [*Yeh et al*., 1996]. This is also true for any attempts to identify hydraulic parameters in the vadose zone. In other words, one should attempt to obtain estimates of hydraulic parameters (such as the natural log of saturated hydraulic conductivity (ln K_s), the natural log of pore-size distribution coefficient (ln α), soil-water pressure head (ψ), and effective saturation (Θ)) that not only preserve their observed values at all sample locations but also satisfy their underlying statistical properties (i.e., mean and covariance). Furthermore, the estimated ln K_s, ln α, ψ, and Θ fields must satisfy the governing flow equation (1), the associated boundary conditions, and the constitutive relationships (3) and (4). In the conditional probability concept, such fields are conditional realizations of the ensemble and many possible realizations of such conditional fields exist. To avoid such a nonuniqueness problem, the goal of this study aims at deriving the expected values of all possible conditional realizations instead of each individual conditional realization.

Consider the case that ln K_s and ln α of a heterogeneous porous medium are stationary stochastic processes, with constant means, $\langle \ln K_s\rangle = F$ and $\langle \ln \alpha\rangle = A$, and perturbations, $f(x)$ and $a(x)$. The angle bracket, $\langle\ \ \rangle$, denotes the ensemble expectation. Similarly, the corresponding soil-water pressure head and effective saturation can be written as $\psi(x) = H(x) + h(x)$ and $\Theta(x) = S(x) + s(x)$, where $H(x) = \langle\psi(x)\rangle$ and $S(x) = \langle\Theta(x)\rangle$ are their means, and $h(x)$ and $s(x)$ are their perturbations. Suppose we have n_f observed saturated hydraulic conductivities, $f^*(x_i)$, where $i = 1, 2, \cdots, n_f$, and n_a observed pore-size distribution coefficient $a^*(x_j)$, where $j = 1, 2, \cdots, n_a$. These data sets will be referred to as the primary information. In addition, we have n_h soil-water pressure measurements, $h^*(x_k)$, where $k = 1, 2, \cdots, n_h$, and n_s effective saturation observations, $s^*(x_l)$, where $l = 1, 2, \cdots, n_s$. These data sets related to the flow process will be called the secondary information.

One possible approach using both primary and secondary information to derive the conditional expectation of ln K_s and ln α is the geostatistical inverse method as presented by *Yeh and Zhang* [1996]. That is,

$$\begin{aligned}Y_c(\mathbf{x}_0) &= F + \sum_{i=1}^{n_f}\beta_i f_i^* + \sum_{k=1}^{n_h}\lambda_k h_k^* + \sum_{l=1}^{n_s}\mu_l s_l^* \\ Z_c(\mathbf{x}_0) &= A + \sum_{j=1}^{n_a}\gamma_j a_j^* + \sum_{k=1}^{n_h}\zeta_k h_k^* + \sum_{l=1}^{n_s}\eta_l s_l^*\end{aligned} \tag{5}$$

where $Y_c(x_0)$ and $Z_c(x_0)$ are cokriged values of ln K_s and ln α at location x_0 using measurements of f^* and a^* at locations x_i, and x_j; measured values of soil-water pressure, h^*, and effective saturation, s^* at locations x_k, and x_l, respectively. The cokriging weights (β, λ, μ, γ, ζ, and η) are derived by minimizing the mean square error (MSE) of cokriging estimates with the knowledge of unconditional covariances of ln K_s, ln α, ψ, and Θ and cross covariances between these variables. In their study, the covariances of h and s, and cross covariances between h and f, h and a, h and s, s and f, s and a, and h and s are approximated by using a numerical first-order approximation approach. They pointed out that since cokriging is a linear estimator, $Y_c(x_0)$ and $Z_c(x_0)$ will be conditional means if and only if that primary and secondary variables are jointly normal and their covariance and cross-covariance functions are known perfectly.

The relationships between f, a, h, and s are nonlinear. Consider one-dimensional vertical flow in an unsaturated porous medium under steady state flow conditions. Assuming that the unsaturated hydraulic conductivity of the medium is described by (3), the natural log of (3) becomes

$$\ln K = F + f - e^{(A+a)}(H + h) \tag{6}$$

If the magnitude of a is small (say, $a \ll 1$), the term, $\exp(a)$, can be approximated by $(1 + a)$. Then, (6) becomes $\ln K \approx F + f - \Lambda(1 + a)(H + h)$, where $\Lambda = \exp(A)$. Hence the governing flow equation can be written in the following form:

$$q = -K(\psi)\left[\frac{d\psi}{dz} + 1\right] = -e^{[F+f+\Lambda(1+a)(H+h)]}\left(\frac{dH}{dz} + 1 + \frac{dh}{dz}\right)$$
$$= -K_g(H)e^{(f+a\Lambda H+\Lambda h+a\Lambda h)}\left[J + \frac{dh}{dz}\right] \tag{7}$$

where $K_g(H) = \exp(F + \Lambda H)$ and J is the mean gradient $(dH/dz + 1)$. Further, one can express the dh/dz term as

$$\frac{dh}{dz} = \frac{q}{K_g(H)}\, e^{-(f+a\Lambda H+\Lambda h+a\Lambda h)} - J \tag{8}$$

On the basis of (8), h is related to f and a in a nonlinear fashion. However, if the sum of all the terms in the exponent is small, (8) can be approximated by

$$\frac{dh}{dz} \approx \frac{q}{K_g(H)}\,[1 - (f + a\Lambda H + \Lambda h + a\Lambda h)] - J \tag{9}$$

Thus h is linearly proportional to f and a. Such a linearized relation (9), being based on small perturbation theory, is valid if and only if the variance of the natural log of unsaturated hydraulic conductivity, $(f + a\Lambda H + \Lambda h + a\Lambda h)$ in (8), is small. As soil becomes less saturated, the variance of unsaturated hydraulic conductivity grows. The nonlinearity becomes stronger [*Yeh et al.*, 1985a, b; *Yeh*, 1989; *Harter and Yeh*, 1996a]. Such a strong nonlinearity in the flow equation implies that in general h will not be normal, and f, a and h will not be jointly normal, even if f and a are normal. In addition, the cross covariances and covariance required in cokriging generally must be derived from a first-order approximation. As a result, the use of linear geostatistical inverse techniques may not produce optimal results even if a large amount of secondary information is incorporated. This problem is bound to be exacerbated if the nonlinearity of the flow equation is stronger. The effect of this problem on the geostatistical inverse approach for saturated flow problems has been demonstrated by *Yeh et al.* [1996].

Besides, cokriged $\ln K_s$, $\ln \alpha$ and ψ fields do not satisfy the continuity equation (1). Suppose we express the conditional random $\ln K_s$, $\ln \alpha$, and ψ fields as the sum of their conditional means and perturbations (i.e., $(\ln K_s)_c = F_c(x) + f_c(x)$; $(\ln \alpha)_c = A_c(x) + a_c(x)$; $\psi_c = H_c(x) + h_c(x)$, where subscript c denotes the conditional value). Taking a logarithm transformation of (1) yields

$$\frac{\partial^2\psi}{\partial x_i^2} + \frac{\partial(\ln K_s + \alpha\psi)}{\partial x_2} + \frac{\partial(\ln K_s + \alpha\psi)}{\partial x_i}\frac{\partial \psi}{\partial x_i} = 0 \tag{10}$$

Substituting the conditional means and perturbations for $\ln K_s$, $\ln \alpha$, and ψ into (10), noticing that for lognormal distribution of the pore-size distribution parameter, $\alpha_c = \exp[A_c(x_1) + a_c(x_1)] = \exp[A_c(x_1)][1 + a_c(x_1) + 0.5a_c^2(x_1) + \cdots]$, and taking the expectation, the exact conditional mean flow equation is

$$\frac{\partial^2 H_c}{\partial x_i^2} + \frac{\partial(F_c + e^{A_c}H_c)}{\partial x_2} + \frac{\partial(F_c + e^{A_c}H_c)}{\partial x_i}\frac{\partial H_c}{\partial x_i}$$
$$+ \left\langle \frac{\partial[e^{A_c}(0.5a_c^2 + \cdots)H_c + e^{A_c}(a_c + 0.5a_c^2 + \cdots)h_c]}{\partial x_2} \right\rangle$$
$$+ \left\langle \frac{\partial[e^{A_c}(0.5a_c^2 + \cdots)H_c + e^{A_c}(a_c + 0.5a_c^2 + \cdots)h_c]}{\partial x_i} \right\rangle \cdot \frac{\partial H_c}{\partial x_i}$$
$$+ \left\langle \frac{\partial[f_c + e^{A_c}h_c + e^{A_c}(a_c + 0.5a_c^2 + \cdots)(H_c + h_c)]}{\partial x_i}\frac{\partial h_c}{\partial x_i} \right\rangle$$
$$= 0 \tag{11}$$

According to (11), the exact conditional mean flow equation consists of two parts. The first part of the equation comprises terms solely related to the conditional mean fields and the other involves the expected value of the products of perturbation terms. This implies that the true conditional mean conductivity (F_c), the pore-size distribution coefficient (A_c), and the head (H_c) do not satisfy the mass balance principle, unless the second part is zero. The second part will be zero only under two conditions: (1) all of the head values in the flow domain are known exactly (i.e., $h_c(x)$ is zero everywhere) or (2) all of the $\ln K_s$ and $\ln \alpha$ values are specified such that their perturbations are zero.

Even if all heads are known exactly, the cokriged $\ln K_s$ and $\ln \alpha$ fields are not necessarily equal to coconditional mean fields (F_c and A_c). Unless both cokriged $\ln K_s$ and $\ln \alpha$ fields and the head field satisfy the flow equation (10). Specifically, the head field derived from solving (10) with the cokriged $\ln K_s$ and $\ln \alpha$ fields will not agree with the observed head field. This discrepancy is attributed to the fact that cokriging assumes a linear relationship between f, a, h, and s. Thus Y_c and Z_c in (5) are merely approximated coconditional mean fields. To derive true coconditional mean $\ln K_s$, $\ln \alpha$, and ψ fields, the nonlinearity between $\ln K_s$, $\ln \alpha$, and ψ must be included in the estimation procedure. In cases where measurements of $\ln K_s$, $\ln \alpha$, and ψ are limited, an inverse model that attempts to derived conditional mean parameters directly, the conditional mean flow equation (11) should be employed.

Iterative Geostatistical Inverse Algorithm

Successive Linear Estimator

Our proposed iterative approach attempts to derive the coconditional mean $\ln K_s$, $\ln \alpha$, ψ, and Θ fields which not only honor the measurements at their sample locations but also satisfy governing flow equation (1). Since the terms in the second part of (11) cannot be evaluated at this moment, we will focus on the development of an iterative geostatistical inverse method that incorporates the nonlinear relations between $\ln K_s$, $\ln \alpha$, and ψ. By considering the nonlinearity, we hope that using the same set of secondary information, this approach will reveal more detailed spatial variation of the primary parameters than the linear (or noniterative) geostatistical inverse method. Although estimated fields from our approach are not necessarily the true coconditional means, they may be called the coconditional effective $\ln K_s$, $\ln \alpha$, ψ, and s fields in the sense they satisfy the mass balance principle. They will be close to the coconditional means if the variance of unsaturated hydraulic conductivity is small (i.e., the magnitude of the second part in (11) is small) or if the amount of secondary information is large.

To accomplish our goal, a successive linear estimator similar to that by *Yeh et al*. [1996] is developed. That is,

$$Y_c^{(r+1)}(\mathbf{x}_0) = Y_c^{(r)}(\mathbf{x}_0) + \sum_{k=1}^{n_h} \lambda_k(\mathbf{x}_k)[\psi_k^*(\mathbf{x}_k) - \psi_k^{(r)}(\mathbf{x}_k)] + \sum_{l=1}^{n_s} \mu_l(\mathbf{x}_l)[\Theta_k^*(\mathbf{x}_l) - \Theta_l^{(r)}(\mathbf{x}_l)] \tag{12}$$

$$Z_c^{(r+1)}(\mathbf{x}_0) = Z_c^{(r)}(\mathbf{x}_0) + \sum_{k=1}^{n_h} \zeta_k(\mathbf{x}_k)[\psi_k^*(\mathbf{x}_k) - \psi_k^{(r)}(\mathbf{x}_k)] + \sum_{l=1}^{n_s} \eta_l(\mathbf{x}_l)[\Theta_l^*(\mathbf{x}_l) - \Theta_l^{(r)}(\mathbf{x}_l)]$$

where r is the iteration index, and $Y_c^{(r)}$ and $Z_c^{(r)}$ present the estimates of conditional means of ln K_s and ln α at iteration r, respectively. These successive linear estimators are unbiased since

$$E[Y_c^{(r+1)}] = E[Y_c^{(r)}] + \sum_{k=1}^{n_h} \lambda_k E[\psi_k^* - \psi_k^{(r)}] + \sum_{l=1}^{n_s} \mu_l E[\Theta_l^* - \Theta_l^{(r)}] = F \tag{13}$$

$$E[Z_c^{(r+1)}] = E[Z_c^{(r)}] + \sum_{k=1}^{n_h} \zeta_k E[\psi_k^* - \psi_k^{(r)}] + \sum_{l=1}^{n_s} \eta_l E[\Theta_l^* - \Theta_l^{(r)}] = A$$

If $r = 0$, $Y_c^{(0)}$ and $Z_c^{(0)}$ correspond to the cokriged ln K_s and ln α fields from (5), respectively. If $r > 0$, new estimates are obtained by adding the weighted sums of $[\psi^* - \psi^{(r)}]$ and $[\Theta^* - \Theta^{(r)}]$ at sample locations to the estimates at the previous iteration. The ψ^* and Θ^* denote the soil-water pressure head and effective saturation values observed at the sample locations. The corresponding simulated soil-water pressure head and effective saturation values, based on ln K_s and ln α fields estimated from the previous iteration, are $\psi^{(r)}$ and $\Theta^{(r)}$. The λ_k, μ_l, ζ_k and η_l are weighting coefficients.

The weighting coefficients vary with iterations. At each iteration, they are determined in a way similar to that in the cokriging technique to ensure the minimal MSE of the estimates, that is,

$$E\{[\ln K_s - Y_c^{(r+1)}]^2\} = \min \qquad E\{[\ln \alpha - Z_c^{(r+1)}]^2\} = \min \tag{14}$$

More specifically, the MSE of the estimates $Y_c^{(r+1)}$, is

$$\begin{aligned} E\{[\ln K_s - Y_c^{(r+1)}]^2\} &= E\left\{\left[\ln K_s - Y_c^{(r)} - \sum_{k=1}^{n_h} \lambda_k^{(r)}(\psi_k^* - \psi_k^{(r)}) - \sum_{l=1}^{n_s} \mu_l^{(r)}(\Theta_l^* - \Theta_l^{(r)})\right]^2\right\} \\ &= E\left\{\left[y^{(r)} - \sum_{k=1}^{n_h} \lambda_k^{(r)} h_k^{(r)} - \sum_{l=1}^{n_s} \mu_l^{(r)} s_l^{(r)}\right]^2\right\} \\ &= R_{yy}^{(r)} + \sum_{k_i=1}^{n_h}\sum_{k_j=1}^{n_h} \lambda_{k_i}^{(r)}\lambda_{k_j}^{(r)} R_{hh}^{(r)} + \sum_{l_i=1}^{n_s}\sum_{l_j=1}^{n_s} \mu_{l_i}^{(r)}\mu_{l_j}^{(r)} R_{ss}^{(r)} - 2\sum_{k=1}^{n_h} \lambda_k^{(r)} R_{yh}^{(r)} \\ &\quad - 2\sum_{l=1}^{n_s} \mu_l^{(r)} R_{ys}^{(r)} + 2\sum_{k=1}^{n_h}\sum_{l=1}^{n_s} \lambda_k^{(r)}\mu_l^{(r)} R_{hs}^{(r)} \end{aligned} \tag{15}$$

where $y^{(r)}$, $h^{(r)}$, and $s^{(r)}$ are the residuals representing the differences between the true fields and the estimated conditional mean fields. Similarly, the MSE associated with $Z_c^{(r+1)}$ can be written as

$$\begin{aligned} E\{[(\ln \alpha)^* - Z_C^{(r+1)}]^2\} &= E\left\{\left[(\ln \alpha)^* - Z_C^{(r)} - \sum_{k=1}^{n_h} \zeta_k^{(r)}(\psi_k^* - \psi_k^{(r)}) - \sum_{l=1}^{n_s} \eta_l^{(r)}(\Theta_l^* - \Theta_l^{(r)})\right]^2\right\} \\ &= E\left\{\left[z^{(r)} - \sum_{k=1}^{n_h} \zeta_k^{(r)} h_k^{(r)} - \sum_{l=1}^{n_s} \eta_l^{(r)} s_l^{(r)}\right]^2\right\} \\ &= R_{zz}^{(r)} + \sum_{k_i=1}^{n_h}\sum_{k_j=1}^{n_h} \zeta_{k_i}^{(r)}\zeta_{k_j}^{(r)} R_{hh}^{(r)} + \sum_{l_i=1}^{n_s}\sum_{l_j=1}^{n_s} \eta_{l_i}^{(r)}\eta_{l_j}^{(r)} R_{ss}^{(r)} - 2\sum_{k=1}^{n_h} \zeta_k^{(r)} R_{zh}^{(r)} \\ &\quad - 2\sum_{l=1}^{n_s} \eta_l^{(r)} R_{zs}^{(r)} + 2\sum_{k=1}^{n_h}\sum_{l=1}^{n_s} \zeta_k^{(r)}\eta_l^{(r)} R_{hs}^{(r)} \end{aligned} \tag{16}$$

where R_{yy}, R_{yh}, R_{ys}, R_{zz}, R_{zh}, R_{zs}, R_{hh}, R_{ss}, and R_{hs} are covariances and cross covariances of the residuals. They may be considered as approximated conditional covariances at the iteration, r.

Minimization of (15) results in a system of equations for determining coefficients, λ_k and μ_l.

$$\sum_{i=1}^{n_h} \lambda_i^{(r)} R_{hh}^{(r)}(\mathbf{x}_k, \mathbf{x}_i) + \sum_{j=1}^{n_s} \mu_j^{(r)} R_{hs}^{(r)}(\mathbf{x}_l, \mathbf{x}_j) = R_{yh}^{(r)}(\mathbf{x}_k, \mathbf{x}) \qquad k = 1, 2, \cdots, n_h \tag{17}$$

$$\sum_{i=1}^{n_h} \lambda_i^{(r)} R_{hs}^{(r)}(\mathbf{x}_l, \mathbf{x}_i) + \sum_{j=1}^{n_s} \mu_j^{(r)} R_{ss}^{(r)}(\mathbf{x}_l, \mathbf{x}_j) = R_{ys}^{(r)}(\mathbf{x}_l, \mathbf{x}) \qquad l = 1, 2, \cdots, n_s$$

Similarly, system of equations for determining coefficients ζ_k and η_l can be derived as

$$\sum_{i=1}^{n_h} \zeta_i^{(r)} R_{hh}^{(r)}(\mathbf{x}_k, \mathbf{x}_i) + \sum_{j=1}^{n_s} \eta_j^{(r)} R_{hs}^{(r)}(\mathbf{x}_l, \mathbf{x}_j) = R_{zh}^{(r)}(\mathbf{x}_k, \mathbf{x}) \qquad k = 1, 2, \cdots, n_h \tag{18}$$

$$\sum_{i=1}^{n_h} \zeta_i^{(r)} R_{hs}^{(r)}(\mathbf{x}_l, \mathbf{x}_i) + \sum_{j=1}^{n_s} \eta_j^{(r)} R_{ss}^{(r)}(\mathbf{x}_l, \mathbf{x}_j) = R_{zs}^{(r)}(\mathbf{x}_l, \mathbf{x}) \qquad l = 1, 2, \cdots, n_s$$

Once the new cokriging coefficients, λ_k, μ_l, ζ_k, and η_l, are evaluated, $Y_c^{(r+1)}$ and $Z_c^{(r+1)}$ can then be calculated using (12).

As ln K_s and ln α fields are improved progressively, the differences, $(\psi^* - \psi^{(r)})$ and $(\Theta^* - \Theta^{(r)})$ will become smaller than those at the previous iterations. Subsequently, values of Y_c and Z_c stabilize, and the spatial variances of the estimated ln K_s and ln α fields (σ_y^2 and σ_z^2, respectively) gradually approach constant values. To end the iterative process, the absolute value of the differences in σ_y^2 and σ_z^2 between two successive iterations are examined. If the differences are less than prescribed tolerances, the iteration stops. Otherwise, a new ψ field is derived by solving flow equation (1) based on the newly calculated Y_c and Z_c and a new effective saturation field is determined by (4). The residual covariances and cross covariances, R_{yy}, R_{zz}, R_{yh}, R_{ys}, R_{zh}, R_{zs}, R_{hh}, R_{hs}, and R_{ss} are then evaluated and thus the new coefficients and new estimates. This iterative process continues.

Residual Covariances and Cross Covariances

Our iterative approach requires the evaluation of residual covariances and cross covariances, R_{yh}, R_{ys}, R_{zh}, R_{zs}, R_{hh}, R_{hs}, and R_{ss} at each iteration. On the basis of first-order analysis of finite element flow equation, soil-water pressure head at rth iteration can be written as a first-order Taylor series:

$$\psi = \psi_c^{(r)} + h^{(r)} = \mathcal{F}[Y_c^{(r)} + y,\, Z_c^{(r)} + z] \approx \mathcal{F}[Y_c^{(r)},\, Z_c^{(r)}] + \frac{\partial \mathcal{F}}{\partial(\ln K_s)}\bigg|_{(Y_c,Z_c)}^{(r)} y^{(r)} + \frac{\partial \mathcal{F}}{\partial(\ln \alpha)}\bigg|_{(Y_c,Z_c)}^{(r)} z^{(r)} \tag{19}$$

where $\mathcal{F}$ represents the finite element analogue of (10). The first-order approximation of the residual of soil-water pressure head $h^{(r)}$ then becomes

$$h^{(r)} \approx \frac{\partial \mathcal{F}}{\partial(\ln K_s)}\bigg|_{(Y_c,Z_c)}^{(r)} y^{(r)} + \frac{\partial \mathcal{F}}{\partial(\ln \alpha)}\bigg|_{(Y_c,Z_c)}^{(r)} z^{(r)} = J_{(hy)}^{(r)} y + J_{(hz)}^{(r)} z \tag{20}$$

where $J_{(hy)}$ and $J_{(hz)}$ are the derivatives (or sensitivities) of soil-water pressure head with respect to ln K_s and ln α, respectively. These derivatives are determined using an adjoint sensitivity analysis subject to boundary conditions [*Zhang*, 1996; *Yeh and Zhang*, 1996]. From (20), the residual covariance of $h^{(r)}$ and residual cross covariances between $h^{(r)}$ and $y^{(r)}$, $h^{(r)}$, and $z^{(r)}$ can be determined (assuming ln K_s and ln α are uncorrelated) as

$$\begin{aligned} R_{hh}^{(r)}(x_i, x_j) &\approx J_{(hy)}^{(r)} R_{yy}^{(r)}(x_m, x_n)[J_{(hy)}^{(r)}]^T + J_{(hz)}^{(r)} R_{zz}^{(r)}(x_m, x_n)[J_{(hz)}^{(r)}]^T \\ R_{yh}^{(r)}(x_i, x_j) &\approx J_{(hy)}^{(r)} R_{yy}^{(r)}(x_m, x_n) \\ R_{zh}^{(r)}(x_i, x_j) &\approx J_{(hz)}^{(r)} R_{zz}^{(r)}(x_m, x_n) \end{aligned} \tag{21}$$

where i and $j = 1, 2, \cdots, n_h$; m and $n = 1, 2, \cdots, N$ (total number of elements); $J_{(hy)}$ and $J_{(hz)}$ are sensitivity matrices of $n_h \times N$, which are also evaluated using the adjoint state sensitivity approach. The superscript T denotes the transpose.

The sensitivities of effective saturation Θ with respect to ln K_s and ln α are defined as

$$J_{(sy)}^{(r)} = \frac{\partial \Theta}{\partial(\ln K_s)}\bigg|_{(Y_c,Z_c)}^{(r)} \qquad J_{(sz)}^{(r)} = \frac{\partial \Theta}{\partial(\ln \alpha)}\bigg|_{(Y_c,Z_c)}^{(r)} \tag{22}$$

Similarly, residual covariance of effective saturation $s^{(r)}$ and residual cross covariances between $s^{(r)}$ and $y^{(r)}$, $s^{(r)}$, and $z^{(r)}$ can be determined by

$$\begin{aligned} R_{ss}^{(r)}(x_i, x_j) &\approx J_{(sy)}^{(r)} R_{yy}^{(r)}(x_m, x_n)[J_{(sy)}^{(r)}]^T + J_{(sz)}^{(r)} R_{zz}^{(r)}(x_m, x_n)[J_{(sz)}^{(r)}]^T \\ R_{ys}^{(r)}(x_i, x_j) &\approx J_{(sy)}^{(r)} R_{yy}^{(r)}(x_m, x_n) \\ R_{zs}^{(r)}(x_i, x_j) &\approx J_{(sz)}^{(r)} R_{zz}^{(r)}(x_m, x_n) \end{aligned} \tag{23}$$

and the residual cross covariance between $s^{(r)}$ and $z^{(r)}$ is given by

$$R_{hs}^{(r)}(x_i, x_j) \approx J_{(sy)}^{(r)} R_{yy}^{(r)}(x_m, x_n)[J_{(hy)}^{(r)}]^T + J_{(sz)}^{(r)} R_{zz}^{(r)}(x_m, x_n)[J_{(hz)}^{(r)}]^T \tag{24}$$

Notice that the calculation of the residual covariance and cross-covariance functions R_{yh}, R_{ys}, R_{zh}, R_{zs}, R_{hh}, R_{hs}, and R_{ss} requires the knowledge of residual covariances R_{yy} and R_{zz}, which represent the covariances of y and z (or residuals of ln K_s and ln α), respectively. These covariances can be expressed as

$$\begin{aligned} R_{yy}^{(r+1)}(\mathbf{x}_o, \mathbf{x}_p) &= R_{yy}^{(r)}(\mathbf{x}_o, \mathbf{x}_p) - \sum_{k=1}^{n_h} \lambda_k^{(r)} R_{yh}^{(r)}(\mathbf{x}_o, \mathbf{x}_k) - \sum_{l=1}^{n_s} \mu_l^{(r)} R_{ys}^{(r)}(\mathbf{x}_o, \mathbf{x}_l) \\ R_{zz}^{(r+1)}(\mathbf{x}_o, \mathbf{x}_p) &= R_{zz}^{(r)}(\mathbf{x}_o, \mathbf{x}_p) - \sum_{k=1}^{n_h} \zeta_k^{(r)} R_{zh}^{(r)}(\mathbf{x}_o, \mathbf{x}_k) - \sum_{l=1}^{n_s} \eta_l^{(r)} R_{zs}^{(r)}(\mathbf{x}_o, \mathbf{x}_l) \end{aligned} \tag{25}$$

where x_o and x_p are any locations in the domain (o and $p = 1, 2, \cdots, M$; M is the total number of elements), and $\lambda_k^{(r)}$, $\mu_l^{(r)}$, $\zeta_k^{(r)}$, and $\eta_l^{(r)}$ are weighting coefficients at iteration r. If $x_o = x_p$, R_{yy} and R_{zz} correspond to the variances of y and z. If $r = 0$, R_{yy} and R_{zz} are equal to the cokriged covariances of ln K_s and ln α, which are determined according to

$$\begin{aligned} R_{yy}^{(1)}(\mathbf{x}_o, \mathbf{x}_p) &= C_{ff}(\mathbf{x}_o, \mathbf{x}_p) - \sum_{i=1}^{n_f} \beta_i C_{ff}(\mathbf{x}_o, \mathbf{x}_i) - \sum_{k=1}^{n_h} \lambda_k^{(0)} C_{fh}(\mathbf{x}_o, \mathbf{x}_k) - \sum_{l=1}^{n_s} \mu_l^{(0)} C_{fs}(\mathbf{x}_o, \mathbf{x}_l) \\ R_{zz}^{(1)}(\mathbf{x}_o, \mathbf{x}_p) &= C_{aa}(\mathbf{x}_o, \mathbf{x}_p) - \sum_{j=1}^{n_a} \gamma_j C_{aa}(\mathbf{x}_o, \mathbf{x}_j) - \sum_{k=1}^{n_h} \zeta_k^{(0)} C_{ah}(\mathbf{x}_o, \mathbf{x}_k) - \sum_{l=1}^{n_s} \eta_l^{(0)} C_{as}(\mathbf{x}_o, \mathbf{x}_l) \end{aligned} \tag{26}$$

where β_I, $\lambda_k^{(0)}$, and $\mu_l^{(0)}$ are cokriging coefficients for ln K_s; γ_j, $\zeta_k^{(0)}$, and $\eta_l^{(0)}$ are coefficients for ln α used in (5). C_{ff} and C_{aa} denote unconditional covariances of ln K_s and ln α, which are assumed to be given. C_{fh}, C_{fs}, C_{ah}, and C_{as} are the unconditional cross-covariances between ln K_s, ln α, ψ, and Θ. They are derived from the first-order analysis similar to (21), (22), (23), and (24).

Condition numbers of matrix equations (17) and (18) can be large if the number of measurements of soil-water pressure and effective saturation is large. Truncation errors can thus be amplified and affect the estimation procedure. To avoid this problem, two relaxation terms, ε and ν, are added to the diagonals of the matrices in (17) and (18) during the iteration. That is,

$$\begin{aligned} \sum_{i=1}^{n_h} \lambda_i R_{hh}(\mathbf{x}_k, \mathbf{x}_i) + \sum_{j=1}^{n_s} \mu_j R_{hs}(\mathbf{x}_l, \mathbf{x}_j) + \varepsilon^{(r)} \lambda_k &= R_{yh}(\mathbf{x}_k, \mathbf{x}) \qquad k = 1, 2, \cdots, n_h \\ \sum_{i=1}^{n_h} \lambda_i R_{hs}(\mathbf{x}_l, \mathbf{x}_i) + \sum_{j=1}^{n_s} \mu_j R_{ss}(\mathbf{x}_l, \mathbf{x}_j) + \nu^{(r)} \mu_l &= R_{ys}(\mathbf{x}_l, \mathbf{x}) \qquad l = 1, 2, \cdots, n_s \end{aligned} \tag{27}$$

$$\sum_{i=1}^{n_h} \zeta_i R_{hh}(\mathbf{x}_k, \mathbf{x}_i) + \sum_{j=1}^{n_s} \eta_j R_{hs}(\mathbf{x}_l, \mathbf{x}_j) + \varepsilon^{(r)}\zeta_k = R_{zh}(\mathbf{x}_k, \mathbf{x}) \qquad k = 1, 2, \cdots, n_h \tag{28}$$

$$\sum_{i=1}^{n_h} \zeta_i R_{hs}(\mathbf{x}_l, \mathbf{x}_i) + \sum_{j=1}^{n_s} \eta_j R_{ss}(\mathbf{x}_l, \mathbf{x}_j) + \nu^{(r)}\eta_l = R_{zs}(\mathbf{x}_l, \mathbf{x}) \qquad l = 1, 2, \cdots, n_s$$

In general, large values of ε and ν reduce the condition numbers of the matrices and oscillations during iterations but they decrease the convergence rate. On the other hand, small values of these relaxation terms can lead to a rapid convergence of the iterative procedure. Nevertheless, they may result in numerical instability and in turn the divergence of the solution in the cases of highly heterogeneous media or in the cases where a large amount of secondary information is used. To avoid these problems, the ε and ν values are assigned dynamically. They are set to be a prescribed fraction of the maximum values of $R_{hh}(x_k, x_k)$ and $R_{ss}(x_l, x_l)$ at each iteration. Since the values of $R_{hh}(x_k, x_k)$ and $R_{ss}(x_l, x_l)$ decreases as the iteration proceeds, the values of ε and ν decrease accordingly. These relaxation terms do not represent the measurement errors as used in cokriging [e.g., *Dietrich and Newsam*, 1989] but merely a technique to control the numerical instability [*Yeh et al.*, 1996].

Numerical Experiments

As mentioned previously, a detailed characterization of the vadose zone is a difficult and costly task. As a result, few large-scale field experiments have focused on the characterization of hydraulic properties of the vadose zone in the past. The Las Cruces experiments [*Wierenga et al.*, 1989] provided a large number of measurements of water release curves but no direct measurements of unsaturated hydraulic conductivity. In addition, ψ and Θ data sets were collected under transient conditions which are not suitable for use in our steady flow model. Hence assessment of our inverse method for identifying hydraulic parameters has to rely on numerical experiments. Nevertheless, numerical experiments are always the first and necessary step for testing any inverse models.

The numerical experiments in our study consider steady state nonuniform flows in two-dimensional hypothetical vadose zones. The domain of the vadose zones is a 7 × 7 m vertical plane which is discretized uniformly into 35 × 35 finite elements with $dx = dy = 20$ cm. The ln K_s and ln α values for each element are generated using a random field generator [*Gutjahr*, 1989], assuming correlation scales for both ln K_s and ln α are 300 and 100 cm in the horizontal and vertical directions, respectively. In addition, ln K_s and ln α are assumed independent of each other. The left and right boundaries of the flow domain are defined as impermeable, and the lower boundary is defined as water table. The central 10 nodes of the upper boundary are set to be a prescribed head boundary, while the remaining parts of the top boundary are specified as no flux boundaries. Once the hypothetical vadose zone is generated, a finite element model [*Yeh et al.*, 1993] is used to solve the primary flow problem (1) with the aid of initial guess solution [*Harter and Yeh*, 1993; *Zhang*, 1996] to obtain the soil-water pressure head ψ and effective saturation Θ fields.

Plate 1. Spatial distributions of (a) ln K_s, (b) ln α, (c) ψ, and (d) Θ in a hypothetical vadose zone (case 2).

These perfectly known ln K_s, ln α, ψ, and Θ fields are then regarded as the real-world analogues (true fields) where measurements of the soil parameters and flow processes are taken. Plate 1 shows the hypothetical ln K_s, ln α, ψ, and Θ fields corresponding to case 2 in our study (see Table 1). Twelve ln K_s and ln α values ($n_f = n_a = 12$) were sampled at a 4 × 3 uniform grid over the entire domain as our primary information (Plates 1a and 1b). The circles in Plates 1a and 1b indicate the location of the samples. The secondary information, soil-water pressure head values, was then taken from an 8 × 8 uniform grid, resulting in a total of 64 soil-water pressure head measurements ($n_h = 64$) (Plate 1c). Similarly, a total of 49 sampled Θ values ($n_s = 49$) was obtained from a 7 × 7 uniform sampling grid (Plate 1d).

To test our iterative approach, a total of 16 cases reflecting different soil parameters and different flow conditions (different prescribed head value at the upper boundary) was examined. Statistical properties (mean value of ln α, variances of ln K_s and ln α) of the soils and the prescribed boundary heads in these cases are tabulated in Table 1. The mean value of ln K_s

Table 1. Statistical Properties of Soils and Boundary Conditions for the Numerical Experiments

Case	Variance of ln K_s, σ_f^2	Variance of ln α, σ_a^2	Geometric Mean of $\alpha\Gamma$, m^{-1}	Prescribed Head at Upper Boundary H, m
1	1.0	0.1	1.0	−1.0
2	1.0	0.1	1.0	−3.0
3	1.0	0.1	1.0	−5.0
4	4.0	0.1	1.0	−1.0
5	4.0	0.1	1.0	−3.0
6	4.0	0.1	1.0	−5.0
7	0.1	0.1	1.0	−1.0
8	0.1	0.1	1.0	−3.0
9	0.1	0.1	1.0	−5.0
10	1.0	0.4	1.0	−1.0
11	1.0	0.4	1.0	−3.0
12	1.0	0.4	1.0	−5.0
13	1.0	0.01	1.0	4.0
14	1.0	0.01	1.0	−3.0
15	1.0	0.01	1.0	−5.0
16	1.0	1.0	0.1	−3.0

for all the cases is specified as -4 m/h. Notice that the magnitude of the mean value does not affect our inverse method since the flow condition is steady.

Two quantitative criteria were used to evaluate the performance of both the noniterative and the iterative approaches. They are

$$Q_1 = \frac{1}{N}\left|\sum_{i=1}^{N}(w_{oi} - w_{ei})\right|$$

$$Q_2 = \frac{1}{N-1}\sum_{i=1}^{N}(w_{oi} - w_{ei})^2 \tag{29}$$

where $|\ \ |$ is the absolute value, and w_{oi} and w_{ei} denote the true and estimated parameter values ($w = \ln K_s$ or $\ln \alpha$) at the ith location, respectively. N is the total number of elements in the domain. Q_1 and Q_2 correspond to the measures of bias (absolute value here) and mean square error of our estimation, respectively, with respect to the true $\ln K_s$ and $\ln \alpha$ fields. The following two quantities were used to quantify the improvement in the estimates due to the use of our iterative approach:

$$P_1 = \frac{Q_{1(\text{Geostatistical})} - Q_{1(\text{Iterative})}}{Q_{1(\text{Geostatistical})}} \times 100\%$$

$$P_2 = \frac{Q_{2(\text{Geostatistical})} - Q_{2(\text{Iterative})}}{Q_{2(\text{Geostatistical})}} \times 100\% \tag{30}$$

where P_1 and P_2 presents percentages of the improvement on the bias and mean square error, respectively.

Contour plots of estimated $\ln K_s$ and $\ln \alpha$ fields for case 2 by both approaches are shown in Plate 2, for visual evaluation of the advantage of our iterative geostatistical approach over the noniterative approach. Comparing these results with the true fields, both noniterative and iterative geostatistical inverse approaches mimic general trends of true $\ln K_s$ and $\ln \alpha$ fields. However, $\ln K_s$ and $\ln \alpha$ fields estimated by the noniterative approach are much smoother than those by the iterative approach and the true fields. On the other hand, the results from the iterative approach reveals some detailed variations of $\ln K_s$ and $\ln \alpha$ fields that resemble those of the true fields. They indicate the improvement due to the incorporation of the nonlinear relationship between f, a, and h. In comparison with the true fields, the estimated fields by our iterative approach are smoother. This smooth nature of our estimates is expected since only a small amount of primary and secondary information are used in the estimation. With such spare data sets (i.e., the stochastic inverse problem [*Yeh et al*., 1996]) the best one can do is to obtain close estimates of the coconditional mean fields which are expected to be smoother than the reality.

Figure 1a illustrates the convergence pattern of our iterative approach, where the maximum values of $[\psi^* - \psi^{(r)}]$ and $[\Theta^* - \Theta^{(r)}]$ at sample locations as a function of the iteration number are depicted. At the zeroth iteration these values correspond to the differences between the observed and simulated ψ and Θ using $\ln K_s$ and $\ln \alpha$ fields estimated by noniterative approach. As indicated in the figure, these differences decrease rapidly as the iteration commences. Behavior of the performance measures (Q_1 and Q_2) for $\ln K_s$ and $\ln \alpha$ as a function of iteration is presented in Figures 1b and 1c. Variances of the estimated conditional mean fields of $\ln K_s$ and $\ln \alpha$ grow as the number of iterations increases but stabilize at approximately

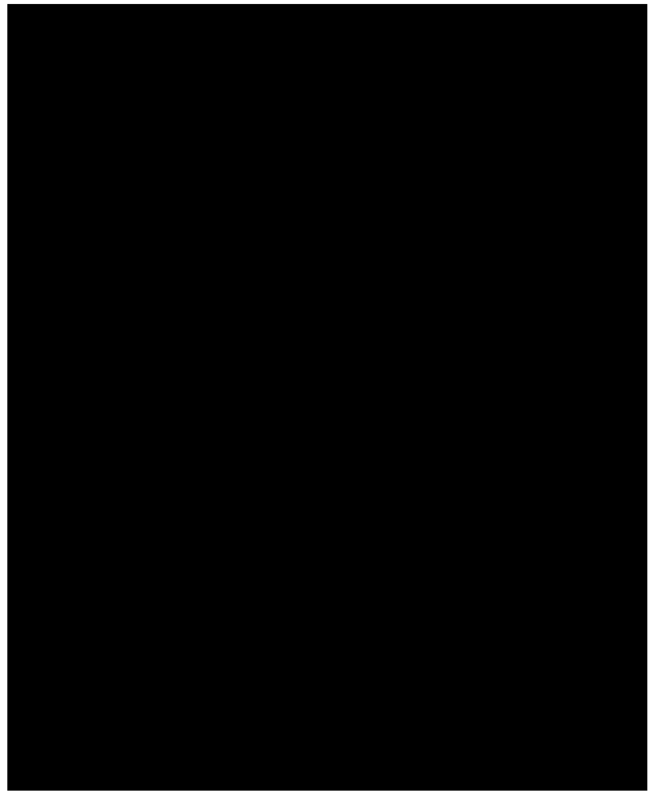

Plate 2. Comparisons of (a, d) true $\ln K_s$ and $\ln \alpha$ fields and (b, e) those estimated by the noniterative and (c, f) the iterative geostatistical inverse approach.

the 20th iteration (Figure 1d). Final values of these variances are 0.74 and 0.041 for σ_f^2 and σ_a^2, respectively. They are greater than those by the noniterative approach and smaller than those of the true fields ($\sigma_f^2 = 1.0$ and $\sigma_a^2 = 0.1$). This result again is consistent with our expectation since our approach attempts to derive the coconditional mean fields, instead of one possible realization of the ensemble of the stochastic processes.

On Tables 2 and 3, the estimated fields by our iterative approach are much better than those by the non-iterative approach in terms of bias and MSE, as suggested by the percentage of improvements. However, our iterative approach produces more biased $\ln \alpha$ fields than the noniterative approach for some cases (such as cases 9 and 15). While the improvement of bias of $\ln \alpha$, and MSE of both $\ln K_s$ and $\ln \alpha$ decreases as the soil becomes less saturated (large negative values of H), the improvement for the bias of $\ln K_s$ varies. The decrease, as the soil becomes less saturated, may be attributed to failure of the first-order approximation of the covariances and cross-covariances in (21)–(24) under dry conditions.

Our iterative approach provides better estimates of unsaturated hydraulic conductivity parameter fields but it requires significantly more computational effort, especially, as the amount of secondary information increases. It took a CPU time of 20 hours (on an IBM RISC/6000/590 workstation with 512-Mb memory) for most of the cases in this study. The adjoint analysis to evaluate the sensitivity of soil-water pressure head with respect to $\ln K_s$ and $\ln \alpha$, and the calculation of error covariances and cross covariances requires a significant amount of CPU time. Recent rapid advances in computer technology and decreases in the price of high-end workstations may ease the computational burden in the future.

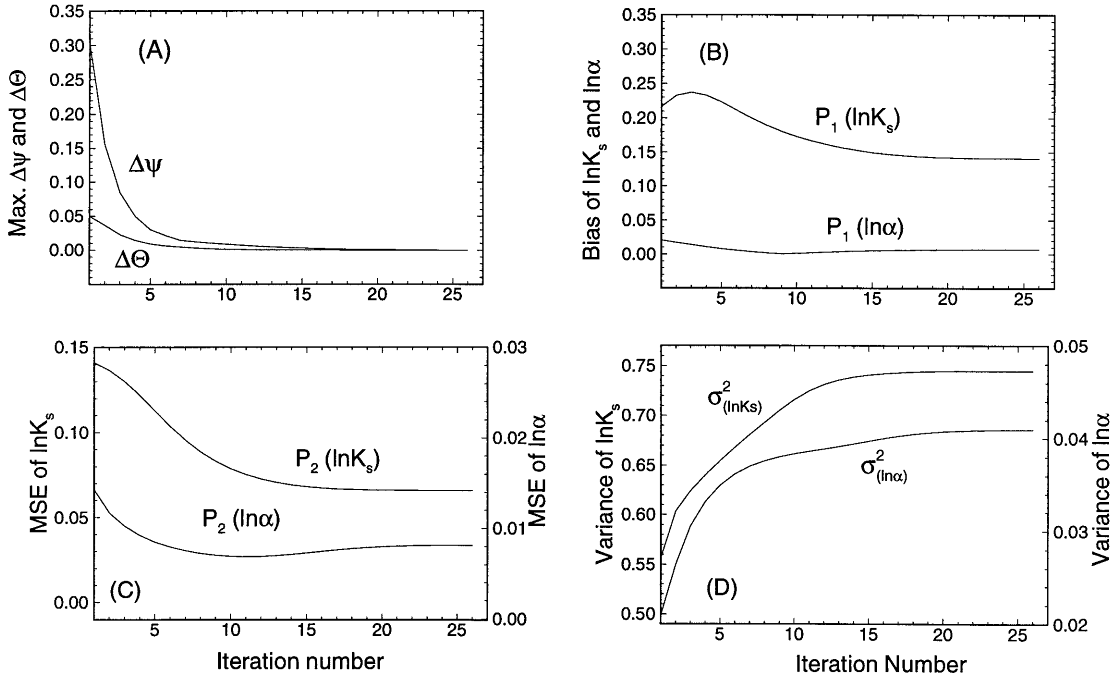

Figure 1. Convergence patterns of the iterative geostatistical inverse approach for case 2.

Finally, while results of the numerical experiments appear interesting, application of this iterative geostatistical inverse approach to field situations remains to be explored. Differences in the sample volume of various sampling devices (e.g., tensiometers, neutron probes, and time domain reflectrometers), methods for in situ measurements of effective saturation are issues to be addressed. In addition, evaluation of the covariance functions of f and a may require many measurements and it will be affected by errors in the measurements [see *Russo and Jury*, 1987a, b]. To alleviate this problem, a maximum likelihood approach used by *Kitanidis and Vomvoris* [1983] can be incorporated in our approach. Also, unsaturated hydraulic property models other than the Gardner and Russo model should be considered.

Conclusions

On the basis of the results of our studies the iterative geostatistical inverse approach using both primary and secondary information is a promising tool for delineating detailed spatial distribution of unsaturated hydraulic heterogeneities. Estimates from the iterative geostatistical inverse approach are better than those derived from noniterative approach. The correlation structure embedded in both approaches ensures

Table 2. Comparison of the Bias of the Estimated ln K_s and ln α Fields From Noniterative Inverse Method and Iterative Inverse Method

Case	Noniterative Inverse: Bias of ln K_s	Noniterative Inverse: Bias of ln α	Iterative Inverse: Bias of ln K_s	Iterative Inverse: Bias of ln α	P_1 of ln K_s, %	P_1 of ln α, %
1	0.1917	0.0261	0.1408	0.0072	26.55	72.41
2	0.1910	0.0069	0.1577	0.0007	17.43	89.86
3	0.1736	0.0012	0.1395	0.0004	19.64	66.67
4	0.3844	0.0297	0.0457	0.0112	88.11	62.16
5	0.4263	0.0058	0.2480	0.0041	41.82	29.31
6	0.4173	0.0012	0.2880	0.0009	30.98	25.00
7	0.0517	0.0269	0.0414	0.0029	19.92	89.21
8	0.0475	0.0064	0.0380	0.0038	20.00	40.63
9	0.0501	0.0029	0.0437	0.0048	12.77	−39.58
10	0.1101	0.0708	0.0223	0.0160	79.74	77.40
11	0.0505	0.0905	0.0308	0.0397	39.01	56.13
12	0.1620	0.0784	0.0710	0.0335	56.17	57.27
13	0.0399	0.0105	0.0267	0.0027	34.83	74.28
14	0.0548	0.0017	0.0104	0.0001	81.02	94.11
15	0.0454	0.0012	0.0001	0.0015	99.78	−25.00
16	0.0695	0.0636	0.0418	0.0029	39.86	95.44

Table 3. Comparison of the Mean Square Errors of Estimated ln K_s and ln α Fields From Noniterative and Iterative Inverse Methods

Case	Noniterative Inverse: MSE ln K_s	Noniterative Inverse: MSE ln α	Iterative Inverse: MSE ln K_s	Iterative Inverse: MSE ln α	P_2 of ln K_s, %	P_2 of ln α, %
1	0.1460	0.0204	0.0659	0.0081	55.48	60.29
2	0.2008	0.0119	0.0931	0.0061	53.64	48.74
3	0.2272	0.0114	0.1077	0.0061	52.60	46.49
4	0.7225	0.0324	0.1970	0.0143	74.50	55.86
5	0.8494	0.0151	0.3641	0.0073	57.13	51.66
6	0.9240	0.0114	0.4918	0.0070	46.77	38.59
7	0.0146	0.0107	0.0088	0.0049	39.73	54.21
8	0.0187	0.0112	0.0107	0.0044	42.78	60.71
9	0.0207	0.0128	0.0109	0.0043	47.34	66.41
10	0.1768	0.0529	0.0753	0.0272	57.41	48.58
11	0.2209	0.0711	0.1316	0.0241	40.43	66.10
12	0.3378	0.0811	0.1957	0.0241	42.07	70.28
13	0.1060	0.0030	0.0471	0.0009	55.57	70.00
14	0.1126	0.0013	0.0498	0.0008	55.77	38.46
15	0.1278	0.0009	0.0636	0.0008	50.23	11.11
16	0.1324	0.0189	0.0587	0.0064	55.66	66.13

our estimates to reflect the spatial structure of the vadose zone. A strong cross correlation between primary and secondary information improves our point estimates. Our iterative method enhances such a cross correlation and in turn, results in better estimates. These estimates are, however, not the coconditional mean fields but merely coconditional effective parameter fields. They preserve the measured values of ln K_s, ln α, ψ, and Θ at the sample locations. Further, the ψ and Θ fields are consistent with the estimated ln K_s and ln α field in the sense that they satisfy the mass balance principle. Although further theoretical development is needed to derive the exact coconditional mean fields and to improve the first-order estimate of the covariances, our study presents an initial attempt to address the complex parameter identification problem in the vadose zone. For many practical problems the noniterative geostatistical inverse approach presented by *Yeh and Zhang* [1996] may be a reasonable tool.

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