Cokriging estimation of the conductivity field under variably saturated flow conditions

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Abstract. A linear estimator, cokriging, was applied to estimate hydraulic conductivity, using pressure head, solute concentration, and solute arrival time measurements in a hypothetical, heterogeneous vadose zone under steady state infiltrations at different degrees of saturation. Covariances and cross-covariances required by the estimator were determined by a first-order approximation in which sensitivity matrices were calculated using an adjoint state method. The effectiveness of the pressure, concentration, and arrival time measurements for the estimator were then evaluated using two statistical criteria, L_1 and L_2 norms, i.e., the average absolute error and the mean square error of the estimated conductivity field. Results of our analysis showed that pressure head measurements at steady state flow provided the best estimation of hydraulic conductivity among the three types of measurements. In addition, head measurements of flow near saturation were found more useful for estimating conductivity than those at low saturations. The arrival time measurements do not have any significant advantage over concentration. Factors such as variability, linearity, and ergodicity were discussed to explain advantage and limitation of each type of data set. Finally, to take advantage of different types of data set (e.g., head and concentration), a computationally efficient estimation approach was developed to combine them sequentially to estimate the hydraulic conductivity field. The conductivity field estimated by using this sequential approach proves to be better than all the previous estimates, using one type of data set alone.

1. Introduction

During the past decades, the cokriging technique has been applied extensively to many studies of subsurface hydrology. For instance, *Kitanidis and Vomvoris* [1983] and *Hoeksema and Kitanidis* [1984] applied the technique to one- and two-dimensional saturated, steady flow problems for estimating hydraulic conductivity of geological media. Using cokriging, *Yates and Warrick* [1987] utilized soil temperature to estimate the spatial distribution of moisture content in the subsurface. *Sun and Yeh* [1992] extended the method to estimate conductivity using information on hydraulic head under transient saturated flow conditions. *Harter and Yeh* [1996b] used the cokriging technique to investigate effects of conditioning using head and conductivity measurements on solute transport in the vadose zone. The technique was also employed by *Yeh and Zhang* [1996] to estimate parameters of unsaturated conductivity based on moisture content and head measurements. *Tong* [1996] applied cokriging to estimate the saturated conductivity of geological media using tracer concentration measurements.

Since cokriging is a linear estimator, it is most suitable for linear systems. For nonlinear problems, as encountered in groundwater hydrology, this linear technique cannot fully utilize the benefit of the secondary information (i.e., pressure head, concentration, and arrival time) unless the variability is small as demonstrated by *Yeh et al*. [1996]. To overcome this problem, *Harvey and Gorelick* [1995] developed a sequential approach for cokriging in which information such as head and solute arrival time was used consecutively to improve the estimates of the heterogeneous conductivity field. On the other hand, *Yeh et al*. [1995, 1996] proposed iterative cokriging techniques for nonlinear systems in which the requirement of unbiasedness and minimum variance were imposed during each iteration. By incorporating the nonlinear relationship between head and conductivity in groundwater flow systems, the estimated conductivity field revealed more detailed heterogeneity than using the linear model and more closely resembled the true field. This iterative approach was further extended to unsaturated flow by *Zhang and Yeh* [1997] to estimate parameters for unsaturated hydraulic conductivity in the vadose zone. Similarly, a quasi-linear geostatistical approach was presented by *Kitanidis* [1995] in an attempt to incorporate the nonlinear relationship between the parameter and secondary information of the subsurface flow system.

In spite of the advance in parameter estimation techniques, a practical question remains regarding what kind of measurements (e.g., head, concentration, or other variables) are most useful for estimating the hydrological parameters. Several attempts to address this issue were carried out in the past. For example, *Yeh and Zhang* [1996] found that pressure head measurements can improve estimates of saturated hydraulic conductivity while moisture content measurements improve estimates of the pore size distribution parameter of unsaturated porous media. Further, the authors reported that the effectiveness of the information depends on the degree of saturation of the medium. *Harvey and Gorelick* [1995] demonstrated that solute arrival time may improve the estimate of hydraulic conductivity for fully saturated porous media when estimates based on heads are not effective. *McLaughlin and Townley* [1996] stated that steady state heads are insensitive to spatial variations in hydraulic conductivity and that estimation may

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not be improved dramatically when more head measurements are included. They suggested that a smaller number of measurements of other variables (e.g., solute concentration) may prove to be more valuable. Nonetheless, a systematic evaluation of advantages and disadvantages of different data sets for variably saturated flow regimes has never been conducted.

While the type of measurement may be important to a parameter estimation procedure, its robustness may be outweighed by the quantity of a different type of measurement. Thus a combination of different types of information may prove to be superior to one type alone. Yet, if all different types of information are used in cokriging, the size of the cokriging matrix can be very large. As a consequence, the solution of the cokriging system can be unstable, and the estimate deteriorates owing to the ill-conditioning of the matrix and poorly formulated problems [*Dietrich and Newsam*, 1989]. Therefore there is a need to develop an approach for stabilizing the cokriging solution.

The goal of this study is twofold: (1) to evaluate the usefulness of head, concentration, and solute arrival time data sets for parameter estimation using cokriging under variably saturated flow regimes; and (2) to develop a sequential approach to increase efficiency of the cokriging technique when a large amount of different types of data sets are used. To accomplish this goal, a first-order Taylor series expansion was adopted to derive the covariance of and cross-covariance functions between hydraulic head, solute concentration, solute arrival time, and hydraulic parameters (i.e., saturated conductivity and the pore size distribution parameter). An adjoint state method was applied to reduce the computational burden during the evaluation of head and concentration sensitivity matrices required in the first-order approximation of the covariances. The performance of cokriging using the three types of data was subsequently evaluated under different flow conditions. Finally, we developed an estimation technique using head and concentration measurements to sequentially estimate the conductivity field, which alleviated instability and other problems associated with the cokriging technique.

2. Methodology

2.1. Equations of Flow and Solute Transport in Variably Saturated Media

In this study, two-dimensional flow in porous media under variably saturated conditions is assumed to be described by

$$[S_s\beta + C_y(\psi)]\,\frac{\partial \psi}{\partial t} = \nabla_{\mathbf{x}} \cdot [K(\psi)\nabla_{\mathbf{x}}(\psi + x_2)] \tag{1}$$

with initial and boundary conditions

$$\psi|_{t=0} = \psi_0, \qquad \psi|_{\Gamma_1} = \psi_p, \qquad K\nabla_{\mathbf{x}}\psi \cdot \mathbf{n}|_{\Gamma_2} = q_b, \tag{2}$$

where ψ is the pressure head, ψ_0 is the initial pressure head, S_s is the specific storage, β is the index for saturation (which is zero if $\psi < 0$ and one if $\psi \geq 0$), C_y is the moisture capacity, $\mathbf{x}$ is the spatial coordinate ($\mathbf{x} = \{x_1 x_2\}$ in which x_2 represents the vertical direction positive upward), and t is time. The subscript $\mathbf{x}$, for the gradient operator, will be dropped hereafter for convenience. Dirichlet boundary conditions are represented by Γ_1 on which prescribed head ψ_p is defined, Γ_2 represents Neumann boundary conditions with a boundary flux q_b, n is a unit normal vector, and K is the unsaturated conductivity which is related to the pressure head through the exponential model [*Gardner*, 1958]

$$K(\psi) = K_s \exp(\alpha\psi), \tag{3}$$

where K_s and α are the saturated conductivity and the pore size distribution parameter, respectively. On the basis of the exponential model, *Russo* [1988] presented a consistent form of water content-pressure (θ-ψ) relationship

$$\theta = (\theta_s - \theta_r)[\exp(0.5\alpha\psi)(1 - 0.5\alpha\psi)]^{2/(2+b)} + \theta_r, \tag{4}$$

where θ_r is the residual water content and θ_s is the saturated water content. Parameter b is chosen to be zero in this study for mathematical simplicity. The moisture capacity in (1) is then defined as $d\theta/d\psi$.

The transport of a conservative solute in a heterogeneous porous medium under variably saturated conditions is governed by the convection-dispersion equation [*Bear*, 1979]

$$\frac{\partial(\theta C)}{\partial t} = \nabla \cdot (\mathsf{D}\nabla C) - \nabla \cdot (\mathbf{q}C) \tag{5}$$

subject to boundary conditions

$$C|_{t=0} = C_0, \qquad C|_{\Gamma_1} = C_1, \qquad -\mathsf{D}\nabla C \cdot \mathbf{n}|_{\Gamma_2} = \mathbf{q}_s \tag{6}$$

where C is the concentration of solutes, C_0 is the initial concentration distribution, C_1 is the prescribed concentration at Dirichlet boundaries, q_s is the solute flux at the Neumann boundaries, D is the hydraulic dispersion tensor, and $\mathbf{q}$ is the flux vector given by Darcy's law

$$\mathbf{q}_i = -K\,\frac{\partial(\psi + x_2)}{\partial x_i} \qquad i = 1, 2. \tag{7}$$

The dispersion tensor is calculated based on the flux as

$$\mathsf{D}_{ij} = (\alpha_L - \alpha_T)\,\frac{q_i q_j}{|q|} + \alpha_T|q|\delta_{ij} \qquad i, j = 1, 2, \tag{8}$$

where α_L and α_T are the local longitudinal and transverse dispersivity, respectively, δ_{ij} is the Kronecker delta ($\delta_{ij} = 1$ if $i =$ j and 0 otherwise), and $|\mathbf{q}|$ is the magnitude of the Darcy flux.

One way to represent field heterogeneity is to treat the hydraulic parameters in the above mentioned flow and solute transport equations as second-order stochastic random fields [*Yeh*, 1998]. Since spatial variations in the parameters such as S_s, θ_s, θ_r, α_L, and α_T are generally small [*Russo and Bouton*, 1992], the parameters are considered constant in space. Subsequently, we regard only the log-transformed saturated conductivity and the pore size distribution parameter (i.e., $\mathrm{Ln}K_s$ and $\mathrm{Ln}\alpha$) as random fields, consisting of a mean and perturbation. That is, $\mathrm{Ln}K_s = F + \mathbf{f}$ and $\mathrm{Ln}\alpha = A + \mathbf{a}$, in which F and A are the mean values, $E[f]$ and $E[a]$ are zeros, and E[ ] is the expectation. Therefore $C_y = \hat{C}_y + \mathbf{c_y}$, $\psi = H + \mathbf{h}$, $\mathbf{q} = \mathbf{q_m} + \mathbf{q}'$, $C = \hat{C} + \mathbf{c}$, and $\theta = \Theta + \theta'$, where $\hat{C}_y$, H, $\mathbf{q_m}$, $\hat{C}$, and Θ are the mean values and $E[\boldsymbol{c_y}]$, $E[\boldsymbol{h}]$, $E[\boldsymbol{q}']$, $E[\boldsymbol{c}]$, and $E[\theta']$ are zeros.

2.2. The Cokriging Equations

Cokriging is a linear predictor that estimates a random field based on measurements of the primary variable (i.e., hydraulic conductivity) and other secondary variables (i.e., head, concentration, and travel time). For example, if the hydraulic conductivity at a given location is the parameter to be estimated, using the measurements of hydraulic conductivity (primary information) and hydraulic heads at other locations (secondary information), the linear predictor for LnK_s can be written as

$$f_0^* = \sum_{i=1}^{n_f} \boldsymbol{\mu}_{0i} f_i + \sum_{j=1}^{n_h} \boldsymbol{\lambda}_{0j} h_j, \tag{9}$$

where n_f is the number of conductivity measurements, n_h is the number of head measurements, f_0^* represents the predicted LnK_s value at location $\mathbf{x}_0$, f_i and h_j represent measurements of log-conductivity and head at locations $\mathbf{x}_i$ and $\mathbf{x}_j$, respectively, and $\boldsymbol{\lambda}_{0i}$ and $\boldsymbol{\mu}_{0j}$ are cokriging weights for the corresponding locations. Note that f and h are mean-removed measurements, implying that their means are known.

To evaluate the cokriging coefficients, the unbiasedness and minimum estimation variance criteria need to be satisfied. Unbiasedness is automatically satisfied since the means have been removed from both sides of (9). Minimization of the estimation variance leads to the following cokriging equations:

$$\sum_{j=1}^{n_f} \boldsymbol{\mu}_{0j} R_{ff}(\mathbf{x}_i;\, \mathbf{x}_j) + \sum_{k=1}^{n_h} \boldsymbol{\lambda}_{0k} R_{fh}(\mathbf{x}_i;\, \mathbf{x}_k) = R_{ff}(\mathbf{x}_0;\, \mathbf{x}_i) \qquad i = 1,\, n_f$$

$$\sum_{j=1}^{n_f} \boldsymbol{\mu}_{0j} R_{hf}(\mathbf{x}_\ell;\, \mathbf{x}_j) + \sum_{k=1}^{n_h} \boldsymbol{\lambda}_{0k} R_{hh}(\mathbf{x}_\ell;\, \mathbf{x}_k) = R_{hf}(\mathbf{x}_0;\, \mathbf{x}_\ell) \qquad \ell = 1,\, n_h \tag{10}$$

where R_{ff} is the covariance of f, R_{hf} is the cross-covariance between h and f, and R_{hh} is the covariance of head. Calculations of these covariance functions are given later in this paper. Corresponding to (9) and (10), the conditional covariance matrix, ε_{ff}, is then given as

$$\varepsilon_{ff}(\mathbf{x}_0;\, \mathbf{x}_j) = R_{ff}(\mathbf{x}_0;\, \mathbf{x}_j) - \sum_{i=1}^{n_f} \boldsymbol{\mu}_{0i} R_{ff}(\mathbf{x}_i;\, \mathbf{x}_j) - \sum_{k=1}^{n_h} \boldsymbol{\lambda}_{0k} R_{fh}(\mathbf{x}_k;\, \mathbf{x}_j) \qquad j = 1,\, N, \tag{11}$$

where N is the total number of elements. When concentration or data other than head are used to estimate conductivity, similar linear estimators and cokriging equations can be constructed.

The above formulation of the cokriging equations assumes that measurements of parameters and secondary information are precise although in practice they may include measurement errors. This type of error is commonly incorporated in cokriging by adding the variance of the errors to the diagonal terms of the covariance functions of primary and secondary information [*Marsily*, 1986]. The measurement error of a primary variable can be included in the covariance function of the variable as a nugget. The effect of a nugget on the cokriging estimate is that the estimated field is more erratic than the error-free estimate. On the other hand, if measurement errors associated with secondary information (such as head or concentration) are added to the diagonal terms of their autocovariance matrices, the cokriging estimate becomes smoother than the error-free one since less information is extracted from these measurements.

In addition to measurement errors, inappropriate choice of units and redundant data points may cause the cokriging covariance matrix to become ill-conditioned (i.e., have extremely large condition numbers) which may cause the solution of the cokriging estimate to be unstable [*Dietrich and Newsam*, 1989]. To overcome ill-conditioning, a small positive value (acting as a stabilizing term) can be added to the diagonal terms of the covariance matrices of secondary information such as head. Similar to the effect of measurement errors of secondary information, the effect of adding this stabilizing term on the cokriging estimate is smoothing unless an iterative approach is used [*Yeh et al*., 1996; *Zhang and Yeh*, 1997].

2.3. Sequential Approach

The principle of our sequential approach is similar to that used by *Harvey and Gorelick* [1995], but the purpose is different. Our sequential estimation begins with treating the f field, estimated using head measurements (i.e., equation (9)), as a conditional mean f field to solve the flow and transport equations for the corresponding conditional mean concentration field. Subtracting the conditional mean concentration value from the measured concentration value at a sampling location yields the conditional concentration perturbation. The perturbations at all sampling locations are then used to improve the estimation of conductivity using a linear estimator

$$f_0^* = \sum_{j=1}^{n_c} \gamma_{0j} c_j. \tag{12}$$

The coefficients γ_{0j} in the above equation are derived by solving the following system of equations:

$$\sum_{j=1}^{n_c} \boldsymbol{\gamma}_{0j} \varepsilon_{cc}(\mathbf{x}_i;\, \mathbf{x}_j) = \varepsilon_{cf}(\mathbf{x}_0;\, \mathbf{x}_i) \qquad i = 1,\, n_c. \tag{13}$$

The conditional covariance matrix of concentration, $\boldsymbol{\varepsilon}_{cf}$, and the cross-covariance between f concentration, $\boldsymbol{\varepsilon}_{cf}$, in (13) are evaluated using the mean f field and the conditional covariance given by (11).

2.4. Evaluation of First and Second Moments of Head and Concentration

As shown in the previous section, formulation of the linear estimator and the cokriging system equations require knowledge of the first and second moments of the stochastic processes (i.e., means, and covariance of secondary information and the cross-covariance between the primary and secondary variables). A first-order analysis is adopted to evaluate these stochastic moments. Specifically, using symbols for the means and perturbations of variables defined previously, the mean flow and transport equations can be written as

$$[\hat{C}_y(H) + \beta S_s] \frac{\partial H}{\partial t} = e^{F+He^A} \nabla^2 H + e^{F+He^A} \nabla (F + He^A) \cdot \nabla (H + x_2) + O^2(f,\, a,\, h) \tag{14}$$

$$q_m = -K(H,\, A,\, F) \nabla (H + x_2) + O^2(f,\, a,\, h) \tag{15}$$

$$\frac{\partial (\Theta \hat{C})}{\partial t} = \nabla \cdot (\mathsf{D}_m \nabla \hat{C}) - \nabla \cdot (q_m \hat{C}) + O^2(q',\, c), \tag{16}$$

where D_m is the macrodispersion coefficient. The last terms of the equations that represent the second and higher order terms (i.e., the expected values of products of perturbations) were neglected to yield the first-order approximate mean flow and transport equations. Notice that the first-order mean flow and transport equations have the same form as the original flow and transport equations (1) and (5) by recovering K_s and α from F and A. The mean Darcy's flux of (15) is obtained by assuming that the mean conductivity has the exponential form given by (3).

To derive the second moments, the pressure head and concentration fields can be expanded in a Taylor series about the mean values of these parameters. After neglecting the second- and higher-order terms, first-order approximations of the pressure head and concentration are

$$\begin{aligned} \psi &= H + \left(\frac{\partial \psi}{\partial f}\bigg|_{F,A}\right) f + \left(\frac{\partial \psi}{\partial a}\bigg|_{F,A}\right) a \\ C &= \hat{C} + \left(\frac{\partial C}{\partial f}\bigg|_{F,A}\right) f + \left(\frac{\partial C}{\partial a}\bigg|_{F,A}\right) a. \end{aligned} \tag{17}$$

The above equations can also be written in matrix form if the governing equations are discretized by finite difference or finite element methods

$$\begin{aligned} \{\mathbf{h}\} &= J_{hf}|_{F,A}\ \{\mathbf{f}\} + J_{ha}|_{F,A}\{\mathbf{a}\} \\ \{\mathbf{c}\} &= J_{cf}|_{F,A}\{\mathbf{f}\} + J_{ca}|_{F,A}\{\mathbf{a}\}, \end{aligned} \tag{18}$$

where braces indicate the vector of the discretized variable and J is the Jacobian matrix, which represents the derivative of head or concentration with respect to the parameters. Multiplying (18) by transposes of $\{\mathbf{f}\}$, $\{\mathbf{a}\}$, $\{\mathbf{h}\}$, and $\{\mathbf{c}\}$ and taking the expected value on both sides result in

$$\begin{aligned} R_{hf} &= J_{hf} R_{ff} \\ R_{ha} &= J_{ha} R_{aa} \\ R_{hh} &= J_{hf} R_{ff} J_{hf}^T + J_{ha} R_{aa} J_{ha}^T \end{aligned} \tag{19}$$

$$\begin{aligned} R_{cf} &= J_{cf} R_{ff} \\ R_{ca} &= J_{ca} R_{aa} \\ R_{cc} &= J_{cf} R_{ff} J_{cf}^T + J_{ca} R_{aa} J_{ca}^T, \end{aligned} \tag{20}$$

where R_{aa} are the covariance functions of a, R_{ha} are the cross-covariance functions between h and a, R_{cc} is covariance function of concentration, and R_{cf} and R_{ca} are the cross-covariance functions between concentration and f and a, respectively. The cross correlation between f and a is assumed to be zero due to the lack of field data supporting their correlation. More importantly, cases where f and a are uncorrelated represent the worst scenario since any correlation between the two parameters enhances the usefulness of the information regarding either one of these parameters.

Note that this first-order approximation is valid only when the variability of the random variables is small. For cases when the variance is large, a higher-order approximation is needed [*Liedl*, 1994].

2.5. Sensitivity Analysis of Head by the Adjoint State Method

As shown in the previous section, the evaluation of the second moments of head requires the determination of the Jacobian matrices. The calculation of Jacobian matrices is often referred to as a sensitivity analysis, since Jacobian matrices represent the change of head in response to changes in hydraulic parameters. *Li and Yeh* [1998] derived the sensitivity of head with respect to f and a based on the adjoint state method for the case where the initial head is prescribed. In this study, the uncertainty associated with the initial condition will be considered. Following the formulation by *Li and Yeh* [1998], the marginal sensitivity of a performance function P is given by

$$\begin{aligned} \frac{\partial P}{\partial f} = \int_T \int_\Omega \Bigg\{ \frac{\partial G}{\partial f} &+ \bigg[\frac{\partial G}{\partial \psi} - (S_s\beta + C_y) \frac{\partial \phi_1^*}{\partial t} \\ &+ \alpha K \nabla(\psi + x_2) \cdot \nabla \phi_1^* - \nabla \cdot (K \nabla \phi_1^*) \bigg] \phi_1 \\ &+ \frac{\partial K_s}{\partial f} \exp(\alpha\psi) \nabla(\psi + x_2) \cdot \nabla \phi_1^* \Bigg\}\, d\Omega\, dt \\ &+ \int_\Omega (S_s\beta + C_y) \phi_1^* \phi_1\, d\Omega|_{t=N_t} \\ &- \int_\Omega (S_s\beta + C_y) \phi_1^* \phi_1\, d\Omega|_{t=0} \\ &- \int_T \int_\Gamma \frac{\partial q_b}{\partial f} \phi_1^* \cdot \mathbf{n}\, d\Gamma\, dt + \int_T \int_\Gamma K \nabla \phi_1^* \phi_1 \cdot \mathbf{n}\, d\Gamma\, dt, \end{aligned} \tag{21}$$

where T and Θ are time and spatial domains, respectively, ϕ_1 is the state sensitivity $(\partial\psi/\partial f)$, G is the state function to be specified later, and $\phi_1{}^*$ is the adjoint state variable satisfying the adjoint state equation

$$\frac{\partial G}{\partial \psi} - (S_s\beta + C_y) \frac{\partial \phi_1^*}{\partial t} + \alpha K \nabla(\psi + x_2) \cdot \nabla \phi_1^* - \nabla \cdot (K \nabla \phi_1^*) = 0 \tag{22}$$

subject to boundary and terminal conditions

$$\phi_1^*|_{\Gamma_1} = 0, \qquad K \nabla \phi_1^* \cdot \mathbf{n}|_{\Gamma_2} = 0, \qquad \phi_1^*|_{t=N_t} = 0, \tag{23}$$

where Γ represents the boundary surrounding domain R and N_t is the final or terminal time. Equation (22) is then solved backward in time.

The above boundary and terminal conditions for the adjoint state variable cause the second, fourth, and fifth terms of the right-hand side of (21) to vanish. The third term disappears only when the initial head is hydrostatic as shown by *Li and Yeh* [1998]. When the initial head distribution is nonhydrostatic, the third term needs to be incorporated into the sensitivity analysis. To evaluate this term, we assume the initial head satisfies a steady state flow equation

$$\nabla \cdot [K(\psi_0) \nabla(\psi_0 + x_2)] = 0. \tag{24}$$

Following the same procedure given by *Li and Yeh* [1998] (taking the derivative of (24) with respect to $\mathrm{LnK_s}$, applying Green's first identity, multiplying both sides of the equation with an arbitrary function $\phi_0{}^*$, and integrating over the simulation domain), we obtain

$$\int_{\Omega} (-\nabla \cdot (K\nabla \phi_0^*)\phi_0 + (K + K\alpha\phi_0)\nabla(\psi_0 + x_2) \cdot \nabla \phi_0^*)\, d\Omega$$

$$+ \int_{\Gamma} \frac{\partial q_b}{\partial f}\, \phi_0^* \cdot \mathbf{n}\, d\Gamma + \int_{\Gamma} K\nabla \phi_0^* \phi_0 \cdot \mathbf{n}\, d\Gamma = 0, \tag{25}$$

where ϕ_0 is the state sensitivity of initial steady state head. Adding equation (25) to equation (21), taking into account that $\phi_1|_{t=0} = \phi_0$, and setting the coefficient of ϕ_0 equal to zero we have

$$-(S_s\beta + C_y)\phi_1^{*0} + \alpha K\nabla(\psi_0 + x_2) \cdot \nabla \phi_0^* - \nabla \cdot (K\nabla \phi_0^*) = 0 \tag{26}$$

with boundary conditions

$$\phi_0^*|_{\Gamma_1} = 0, \qquad K\nabla \phi_0^* \cdot \mathbf{n}|_{\Gamma_2} = 0. \tag{27}$$

The variable $\phi_1{}^{*0}$ is the transient adjoint state variable at $t = 0$, derived from the solution of (22) with the specification that $G = \psi\delta(\mathbf{x} - \mathbf{x}_k;\ t - t_m)$, where $\mathbf{x}_k$ is the measurement location of head at t_m and δ is the Dirac delta function. Then, the state sensitivity at time t_m is evaluated as

$$\frac{\partial \psi}{\partial f_k} = \frac{\partial P}{\partial f_k} = \int_T\int_{\Omega_k} K\nabla(\psi + x_2) \cdot \nabla \phi_1^*\, d\Omega\, dt$$

$$+ \int_{\Omega_k} K\nabla(\psi_0 + x_2)\nabla \phi_0^*\, d\Omega, \tag{28}$$

where Θ_k is the exclusive subdomain of f_k which is element k in this study since f is defined at each element.

The evaluation of the sensitivity of pressure head with respect to Lnα are identical to equations (22) and (26) However, the state sensitivity is now given by

$$\frac{\partial \psi}{\partial a_k} = \frac{\partial P}{\partial a_k} = \int_T\int_{\Omega_k} K\psi\alpha\nabla(\psi + x_2) \cdot \nabla \phi_1^*\, d\Omega\, dt$$

$$+ \int_{\Omega_k} K\psi_0\alpha\nabla(\psi_0 + x_2) \cdot \nabla \phi_0^*\, d\Omega. \tag{29}$$

Since the adjoint state equations only need to be solved once for f and a, considerable CPU time can be saved for the evaluation of the sensitivities. In contrast to the sensitivities derived by *Li and Yeh* [1998] for the hydrostatic condition, (28) and (29) also include the sensitivity of initial heads with respect to the parameters.

2.6. Sensitivity Analysis of Concentration by the Adjoint State Method

The method for calculating the sensitivity of concentration with respect to hydraulic parameters differs from that of head sensitivity because concentration is not only a function of hydrological parameters but also a function of head. The dependence of concentration on head requires a scheme that couples flow and transport equations to derive the sensitivity of concentration with respect to each parameter. *Sun and Yeh* [1990] presented a self-defined operator that can generate adjoint state equations for this problem. Below, we will follow our approach [*Li and Yeh*, 1998] to generate adjoint state equations and to derive the sensitivity of concentration with respect to the hydrological parameters. The detail of the procedure is given below since it is not completely identical to the procedure used in the head sensitivity analysis.

The performance measure now is defined as

$$P = \int_T\int_{\Omega} G(C, f, a)\, d\Omega\, dt. \tag{30}$$

Taking the derivative of the performance function with respect to any of the parameters (e.g., f) results in the marginal sensitivity of the performance function

$$\frac{\partial P}{\partial f} = \int_T\int_{\Omega} \left(\frac{\partial G}{\partial f} + \frac{\partial G}{\partial C}\frac{\partial C}{\partial f}\right) d\Omega\, dt. \tag{31}$$

Equation (31) requires the evaluation of $\partial C/\partial f$. To do so, we differentiate (5) with respect to f

$$\nabla \cdot \left(\frac{\partial D}{\partial f}\nabla C\right) + \nabla \cdot \left(D\nabla \frac{\partial C}{\partial f}\right) - \nabla \cdot \left(\frac{\partial q}{\partial f}\, C\right)$$

$$- \nabla \cdot \left(q\, \frac{\partial C}{\partial f}\right) - \frac{\partial}{\partial t}\left(\frac{\partial(\theta C)}{\partial f}\right) = 0 \tag{32}$$

in which

$$\frac{\partial D}{\partial f} = \sum_{i=1}^{2} \frac{\partial D}{\partial q_i}\frac{\partial q_i}{\partial f} \tag{33}$$

$$\frac{\partial q_i}{\partial f} = q_i + \alpha q_i\frac{\partial \psi}{\partial f} - K\frac{\partial}{\partial x_i}\left(\frac{\partial \psi}{\partial f}\right). \tag{34}$$

Note that the notation of $\partial D/\partial f$ and $\partial D/\partial q_i$ means taking the derivative of each item in the dispersion tensor with respect to f and q_i. Following the same steps given by *Li and Yeh* [1998], we obtain the marginal sensitivity of concentration with respect to LnK_s

$$\frac{\partial P}{\partial f} = \int_{\Omega}\int_T \left\{\frac{\partial G}{\partial f} + \phi_1\left[CC_y\frac{\partial \phi_2^*}{\partial t} - \alpha F_l q_l\nabla C \cdot \nabla \phi_2^*\right.\right.$$

$$- \frac{\partial}{\partial x_l}(KF_l\nabla C \cdot \nabla \phi_2^*) + \alpha qC \cdot \nabla \phi_2^* + \nabla \cdot (KC\nabla \phi_2^*)$$

$$\left. - (S_s\beta + C_y)\frac{\partial \phi_1^*}{\partial t} + \alpha K\nabla(\psi + x_2) \cdot \nabla \phi_1^* - \nabla \cdot (K\nabla \phi_1^*)\right]$$

$$+ \phi_2\left[\frac{\partial G}{\partial C} + \nabla \cdot (D\nabla \phi_2^*) + q \cdot \nabla \phi_2^* + \theta\frac{\partial \phi_2^*}{\partial t}\right]$$

$$- F_l q_l\nabla C \cdot \nabla \phi_2^* + qC \cdot \nabla \phi_2^*$$

$$\left. + \frac{\partial K_S}{\partial f}\exp(\alpha\psi)\nabla(\psi + x_2) \cdot \nabla \phi_1^*\right\} d\Omega\, dt$$

$$+ \int_{\Gamma}\int_T \frac{\partial(D\nabla C - qC)}{\partial f}\, \mathbf{n} \cdot \phi_2^* d\Gamma\, dt$$

$$+ \int_{\Gamma_{x_1}}\int_T KF_2\nabla C \cdot \nabla \phi_2^*\phi_1\, dx_1\, dt\Big|_{x_2=0}^{x_2=x_{2T}}$$

$$+ \int_{\Gamma_{x_2}} \int_T KF_1 \nabla C \cdot \nabla \phi_2^* \phi_1 dx_2\, dt|_{x_1=0}^{x_1=x_{1T}}$$

$$- \int_\Gamma \int_T D \nabla \phi_2^* \mathbf{n} \phi_2\, d\Gamma dt - \int_\Gamma \int_T KC \nabla \phi_2^* \cdot \mathbf{n} \phi_1\, d\Gamma\, dt$$

$$- \int_T \int_\Gamma \frac{\partial q_b}{\partial f} \phi_1^*\, d\Gamma\, dt + \int_T \int_\Gamma K \frac{\partial \phi_1^*}{\partial x_i} \phi_1\, d\Gamma\, dt$$

$$+ \int_\Omega \theta \phi_2 \phi_2^*|_{t=N_t}\, d\Omega - \int_\Omega \theta \phi_2 \phi_2^*|_{t=0}\, d\Omega$$

$$+ \int_\Omega (S_s\beta + C_y) \phi_1^* \phi_1\, d\Omega|_{t=N_t}$$

$$- \int_\Omega (S_s\beta + C_y) \phi_1^* \phi_1\, d\Omega|_{t=0} - \int C_y C \phi_2^* \phi_1|_{t=N_t}\, d\Omega$$

$$+ \int C_y C \phi_2^* \phi_1|_{t=0}\, d\Omega, \tag{35}$$

where $\phi_1 = \partial\psi/\partial f$, $\phi_2 = \partial C/\partial f$, $F_i = \partial D/\partial q_i$, $\phi_1{}^*$ and $\phi_2{}^*$ are adjoint state variables, and x_{1T} and x_{2T} are the upper boundaries in x_1 and x_2 directions, respectively. Note that (8) of *Li and Yeh* [1998] was also added into (35) due to the dependence of $\partial q/\partial f$ on $\partial\psi/\partial f$. Since ϕ_1 and ϕ_2 are unknowns, we set their coefficients equal to zero, which leads to the following adjoint state equations

$$\frac{\partial G}{\partial C} + \nabla \cdot (D \nabla \phi_2^*) + \mathbf{q} \cdot \nabla \phi_2^* + \theta \frac{\partial \phi_2^*}{\partial t} = 0 \tag{36}$$

$$-\alpha F_l \mathbf{q}_l \nabla C \cdot \nabla \phi_2^* - \frac{\partial}{\partial x_1} (KF_l \nabla C \cdot \nabla \phi_2^*) + \alpha \mathbf{q} C \nabla \phi_2^*$$

$$+ \nabla \cdot (KC \nabla \phi_2^*) + CC_y \frac{\partial \phi_2^*}{\partial t} - (S_s\beta + C_y) \frac{\partial \phi_1^*}{\partial t}$$

$$+ \alpha K \nabla(\psi + x_2) \cdot \nabla \phi_1^* - \nabla \cdot (K \nabla \phi_1^*) = 0 \tag{37}$$

subject to boundary and terminal conditions

$$\begin{gathered} \phi_2^*|_{\Gamma_1} = 0, \qquad \phi_1^*|_{\Gamma_1} = 0 \\ \nabla \phi_2^* \cdot \mathbf{n}|_{\Gamma_2} = 0, \qquad \nabla \phi_1^* \cdot \mathbf{n}|_{\Gamma_2} = 0 \\ \phi_2^*|_{N_T} = 0, \qquad \phi_1^*|_{N_T} = 0. \end{gathered} \tag{38}$$

The boundary terms in (35) vanish automatically as a result of the boundary conditions for the adjoint state equations as well as flow and transport equations. The term in (35) containing state sensitivity ϕ_2 at $t = 0$ is zero since initial concentrations are assumed zero everywhere. Terms containing ϕ_1 have been treated previously in the derivation of head sensitivity. If we choose $G = C(\mathbf{x},t)\delta(\mathbf{x} - \mathbf{x}_0, t - t_m)$, where $\mathbf{x}_0$ is the location of a concentration measurement and t_m is the time at which concentration is measured, we can then solve equations (36) and (37) for $\phi_1{}^*$ and $\phi_2{}^*$. Note that (36) and (37) need to be solved conjunctively in that the solution of (36) generates the load term for (37).

The sensitivity of concentration with respect to f is

$$\frac{\partial P}{\partial f} = \int_{\Omega_k} \int_T [-F_l q_l \nabla C \cdot \nabla \phi_2^* + qC \cdot \nabla \phi_2^*$$

$$+ K \nabla(\psi + x_2) \cdot \nabla \phi_1^*]\, d\Omega\, dt$$

$$+ \int_{\Omega_k} K \nabla(\psi_0 + x_2) \cdot \nabla \phi_0^*\, d\Omega \tag{39}$$

Similarly, the sensitivity with respect to a is given by

$$\frac{\partial P}{\partial a} = \int_{\Omega_k} \int_T [-\alpha\psi F_l q_l \nabla C \cdot \nabla \phi_2^* + \alpha\psi qC \cdot \nabla \phi_2^*$$

$$+ K\alpha\psi \nabla(\psi + x_2) \cdot \nabla \phi_1^*]\, d\Omega\, dt$$

$$+ \int_{\Omega_k} K\alpha\psi_0 \nabla(\psi_0 + x_2) \cdot \nabla \phi_0^*\, d\Omega \tag{40}$$

2.7. Sensitivities of Arrival Times

To define arrival time, we follow approach by *Harvey and Gorelick* [1995] to use the percentage of solutes arrived at a sampling location. If Q is the percentage quantile and τ is the arrival time when quantile Q is reached, the relationship between the two is given by

$$Q = \int_0^\tau C\, dt \Big/ \int_0^\infty C\, dt. \tag{41}$$

Taking the derivative of Q with respect to f and reorganizing, we have the sensitivity of arrival time with respect to f

$$\frac{\partial \tau}{\partial f} = \frac{Q \displaystyle\int_0^\infty \frac{\partial C}{\partial f}\, dt - \int_0^\tau \frac{\partial C}{\partial f}\, dt}{C(\tau)}. \tag{42}$$

Thus the calculation of arrival time sensitivity is now directly related to the calculation of the sensitivity of concentration derived in the above analysis. Similarly, the sensitivity of arrival time with respect to Lnα can be calculated by

$$\frac{\partial \tau}{\partial a} = \frac{Q \displaystyle\int_0^\infty \frac{\partial C}{\partial a}\, dt - \int_0^\tau \frac{\partial C}{\partial a}\, dt}{C(\tau)}. \tag{43}$$

3. Numerical Results

3.1. Case Description

A synthetic porous medium, 40 cm wide in the horizontal direction and 200 cm long in the vertical, was created for the following numerical experiments. It was discretized into 500 finite elements (10 in the horizontal and 50 in the vertical direction). The hydraulic properties of each element (LnK_s and Lnα) were constructed by a random field generator using the fast Fourier transformation technique [*Gutjahr*, 1989]. The random fields were assumed to have an exponential model structure with the correlation scale equal to 40 cm in both horizontal and vertical directions. The means of the saturated

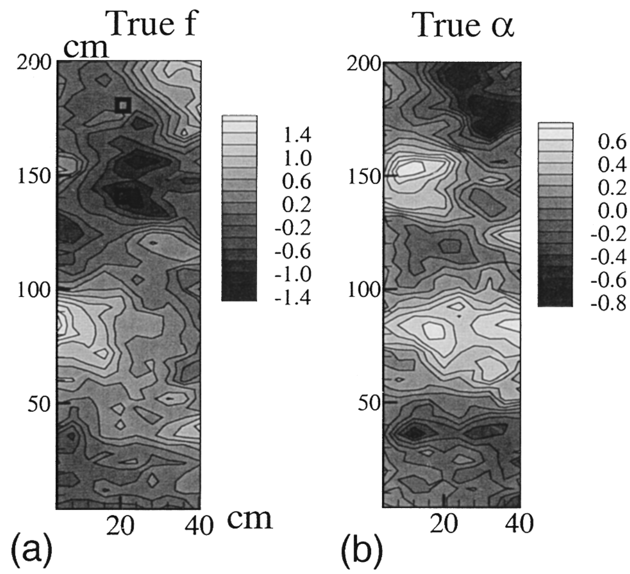

Figure 1. Generated f and a fields.

conductivity and pore size distribution parameter (K_s and α) fields were chosen to be 0.0014 cm/s and 0.1 cm^{-1}, respectively. The variances for the generated f and a, shown in Figure 1, were 0.24 and 0.09, respectively. Note that the parameters, f and a, were assumed to be statistically independent from each other. The values of θ_s and θ_r were specified as 0.4 and 0.0, respectively, and treated as constants in space.

Three steady flow cases were simulated using these synthetic parameter fields. Prescribed heads were set for the upper and lower boundaries of the medium while the left and right boundaries were kept impervious. For case 1, both the upper and lower boundaries were assigned a pressure head value of 30 cm so that the medium was fully saturated and flow was driven by gravity alone. For cases 2, a pressure head value of -10 cm was assigned to the upper and lower boundaries to create the unit mean gradient condition while a head value of -20 cm was used in case 3. Simulated pressure head fields for the three cases are illustrated in Figure 2.

For each of the three flow cases, the evolution of a solute plume, resulting from a pulse of a conservative tracer (released at the location $x = 18$ cm, $z = 178$ cm) was simulated. A prescribed zero concentration condition was specified at the top boundary, and no diffusive flux condition was prescribed for the bottom, right, and left boundaries. For each case, values of 24 and 0.3 cm were used as local dispersivity in the longitudinal and transverse directions, respectively. On the basis of the Courant number criterion, different time step sizes were selected for simulating solute transport for the three cases (i.e., 300, 700, and 1500 s for cases 1, 2, and 3, respectively). The amount of solute injected was therefore different for each case depending on the length of the time step. A snapshot of the concentration distribution at $t = 15{,}000$ s for the saturated flow case is given in Figure 3.

Samples of f were taken at two locations (squares in Figure 1) in the synthetic field while pressure head and concentration were sampled from eighteen locations in the simulated pressure head and concentration fields. The sampling locations for pressure head, concentration, and arrival time are indicated in Figures 2 and 3 by circles. These samples are mean-removed perturbations (i.e., $f = \mathrm{Ln}K_s - F$; $c = C - \hat{C}$, and $h = \psi - H$, in which F is the mean of LnK_s, and $\hat{C}$ and H are mean concentration and pressure head fields evaluated from the first-order mean flow and transport equations with mean parameter values, respectively). At these sampling locations, the 50% arrival times, defined by (41) for both the mean and real concentration fields resulting from the impulse input, were also computed. The estimation of the Lnα field will not be presented in this paper since the general behavior of cokriging in the estimation of Lnα is similar to that of estimating LnK_s.

3.2. Results

Cokriging-estimated f fields, using head measurements in the three different flow cases, are shown in Figures 4a, 4b, and 4c. As illustrated in Figure 4, the general pattern of heterogeneity in the true field (Figure 1a) is captured by cokriging.

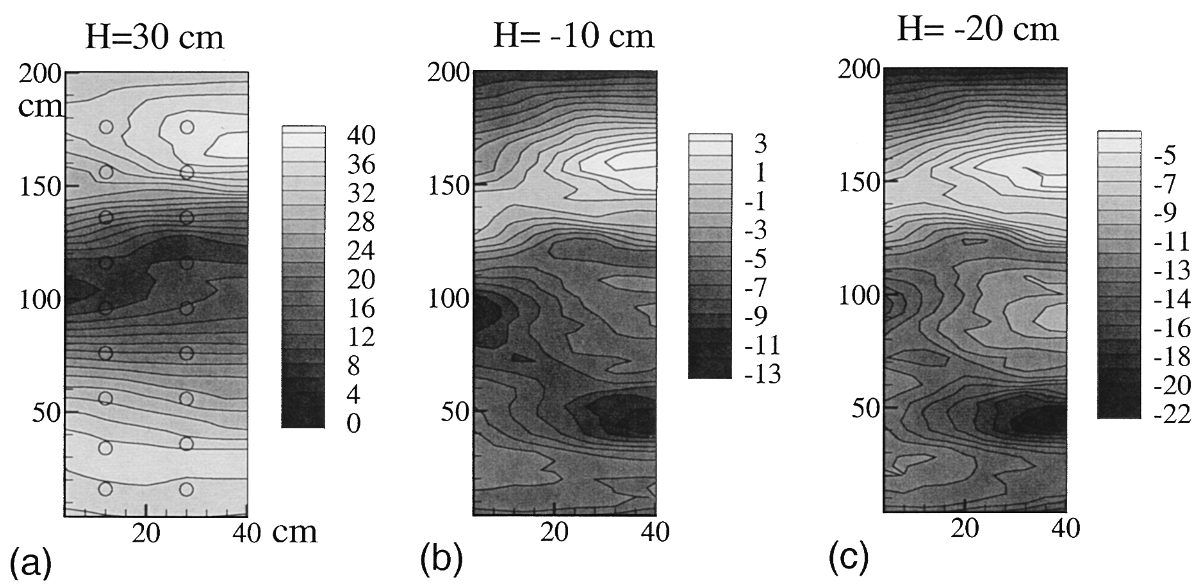

Figure 2. True head distributions for mean pressure heads of 30, -10, and -20 cm, respectively.

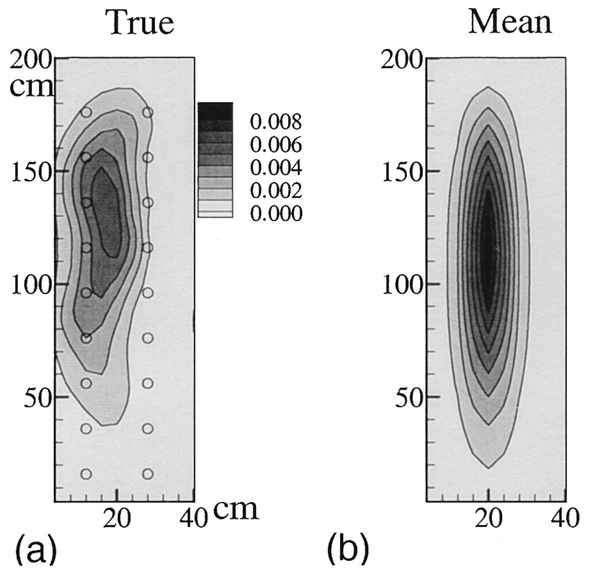

Figure 3. True and mean concentration distributions for the mean pressure head 30 cm.

However, the cokriging estimate loses resolution as the soil becomes drier, especially in the high-permeability zone. In other words, the effect of head information on conditioning the LnK_s field depends on the mean pressure head value: the conditioning effect is stronger when the soil is wetter. A similar result was also reported by *Yeh and Zhang* [1996].

To illustrate the performance of cokriging for the three cases more clearly, scatterplots (i.e., the estimated f versus true f) are shown in Figures 5a, 5b, and 5c. As the soil becomes less saturated, the scattering increases and the trend of data points increasingly deviates more from the 45° line. The performance of cokriging was quantified by the average absolute error, L_1 norm, and the mean square error, L_2 norm

$$L_1 = \frac{1}{N}\sum_{i=1}^{N}|f_{i_{\text{true}}} - f_{i_{\text{cok}}}|$$

$$L_2 = \frac{1}{N}\sum_{i=1}^{N}(f_{i_{\text{true}}} - f_{i_{\text{cok}}})^2, \tag{44}$$

where N is the number of data points on each scatterplot. The values of the two criteria for the three cases are listed in Table 1. The results show that the estimate based on head measurements in the saturated flow yields the smallest L_1 and L_2 norms, while that using heads at -20 cm produces the largest L_1 and L_2 norms. Notice that these measurements reflect the quality of the cokriging estimates for this particular realization of the f field. They are not comparable to the theoretical cokriging estimation variance, which is a minimized ensemble estimation variance, unless the domain size is large. The nonsymmetric scattering of points around the 45° line in these figures is attributed to the small domain size of our estimated conductivity field.

Cokriging estimates in which concentration measurements were used also reproduced the general pattern of the f field but with less detail as compared to that derived from head. From scatterplots of these estimates shown in Figure 6, it is observed that the effect of conditioning using concentration measurements decreases as the soil becomes drier. This observation corroborates the statistics in Table 1. It is important to note, however, that a measurement error term (or a stabilizing term) was added to the diagonal terms of the concentration covariance matrix to stabilize the solution. If it had not been added, the cokriging estimate would exhibit anomalies (i.e., extreme values larger than the maximum value or smaller than the minimum value of the true f field). This measurement error was chosen to be 1–2% of the largest concentration variance among all the concentration measurements. The statistics listed in Table 1 and the scatterplots in Figure 6 are therefore

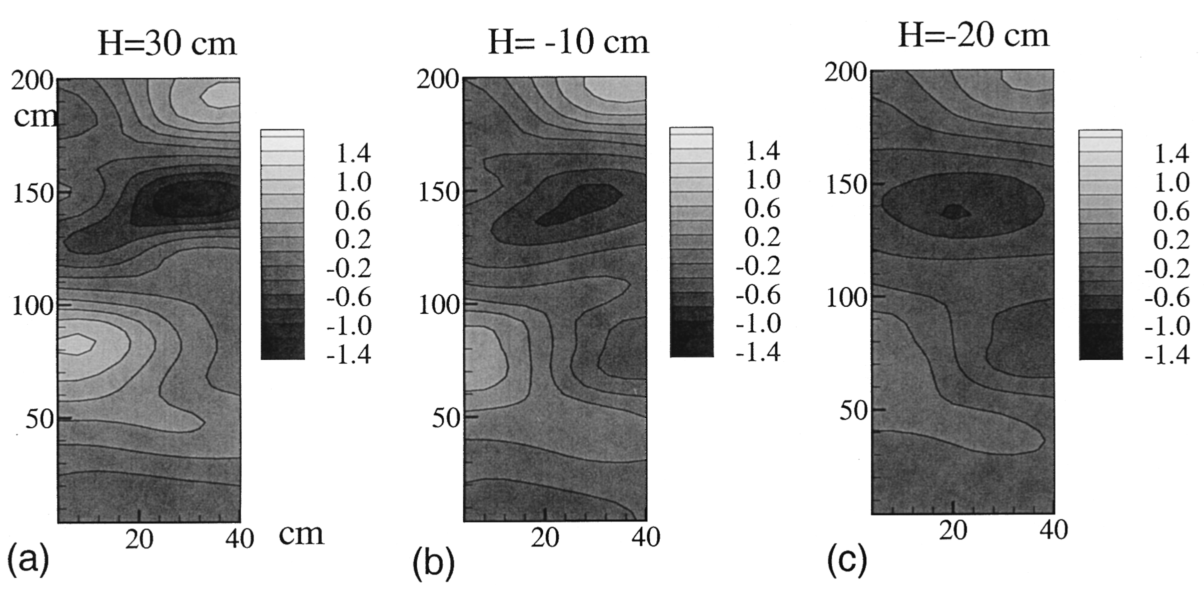

Figure 4. Estimated f fields using head and f measurements for mean pressure heads of 30, -10, and -20 cm, respectively.

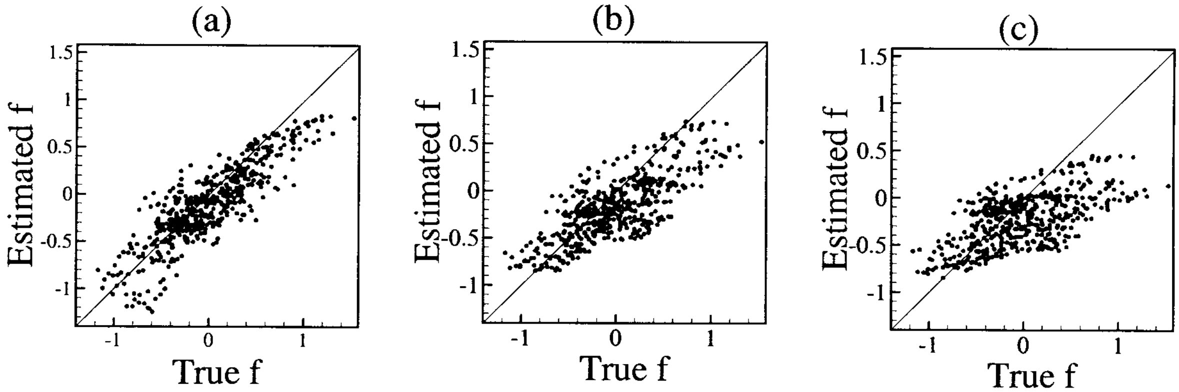

Figure 5. Scatterplot of true f versus estimated f using measurements of f and head for mean pressure heads of 30, -10 cm, and -20 cm.

less indicative of the conditioning effect since they vary with the amount of measurement errors added.

Similar to the cokriging estimation in which measurements of solute concentration were used, the cokriging estimation using arrival time measurements preserved the major features of f field as well. Figure 7 shows the scatterplot of this estimation using the arrival time of 50% quantile measured at the 18 sampling locations in the saturated flow case. The statistics in Table 1 indicate no significant advantage in using arrival time data to estimate conductivity over concentration. The only advantage for using arrival time data appears to be that there was no need to use the stabling term.

While the above cokriging estimation considered only one type of secondary information (either head or concentration or arrival time), the sequential approach developed in this study can be used to incorporate both head and concentration measurements in a consecutive manner. In other words, we first use the f field estimated using head measurements (Figure 4a) as a conditional mean field to determine the conditional mean concentration (Figure 8). Compared to the unconditional mean concentration field shown in Figure 3b, the conditional mean concentration field in Figure 8 is much closer to the true concentration distribution (Figure 3a). After subtracting the conditional mean concentration from the observed true concentration at the eighteen sampling locations, the conditional concentration perturbations are used to estimate hydraulic conductivity using equation (12). The result of this sequential estimate of the conductivity field is shown in Figure 9 and the corresponding scatterplot is given in Figure 10. Compared to the estimates using either head or concentration alone (Figure 5 and 6, respectively), the estimate from the sequential approach resembles the true field more closely. The statistics in Table 1 further quantify this resemblance. No stabilizing term was needed to obtain a well-conditioned matrix during the sequential estimation procedure.

Table 1. Statistics of Estimated f Using Different Measurements

	L_1 Norm	L_2 Norm
Head at $H = 30$ cm	0.22	0.07
Head at $H = -10$ cm	0.28	0.12
Head at $H = -20$ cm	0.35	0.20
Concentration at $H = 30$ cm	0.38	0.21
Concentration at $H = -10$ cm	0.36	0.22
Concentration at $H = -20$ cm	0.46	0.36
Arrival time at $H = 30$ cm	0.36	0.20
Sequential estimate at $H = 30$ cm	0.18	0.052

4. Discussion

Our results show that L_1 and L_2 norms for f estimates using head measurements increase as the soil becomes drier. These increases can be ascribed to the decrease in cross-correlation between head and conductivity as the soil becomes drier, and the increase in variability of head, which subsequently reduces the correlation between head and conductivity.

The same explanation applies to the performance of cokriging using concentration measurements as the medium becomes less saturated. However, several additional issues must be discussed regarding the case of using concentration measurements. At early times of the solute transport process, as in the case studied here, a solute plume generally does not encounter sufficient heterogeneity of the aquifer and does not reach the well-developed Fickian regime. Consequently, the plume predicted by the ensemble mean transport equation may not resemble the true plume. Specifically, the shape and the location of the calculated mean plume (Figure 3b) may be quite different from those of the observed one (Figure 3a). Furthermore, the calculated mean plume assumes the validity of the mean flow and convective-dispersive equations (equations (14)–(16)) and the existence of the effective parameters (such as effective conductivity and macrodispersivity) that rely on the ergodicity assumption. In other words, the ensemble mean plume can be highly skewed [e.g., *Harter and Yeh*, 1996a, Figure 1] and very different from the one shown in Figure 3b if the ergodicity is not met. Because of the lack of ergodicity, the variance of concentration perturbation of the plume was very large and the estimation using concentration measurements was not satisfactory. Note that although the flow analysis also assumes ergodicity, the time to reach ergodicity generally is greater for concentration than pressure head, since head, especially in the saturated flow, is more diffusive than concentration [*Yeh*, 1998].

The problems associated with the ergodicity assumption related to the mean concentration field, however, diminishes when the field is conditioned on the measurements of head and conductivity. This can be seen by comparing Figures 3a and 8, in which the conditioned mean plume distribution becomes similar to that of the true plume. Consequently, the concen-

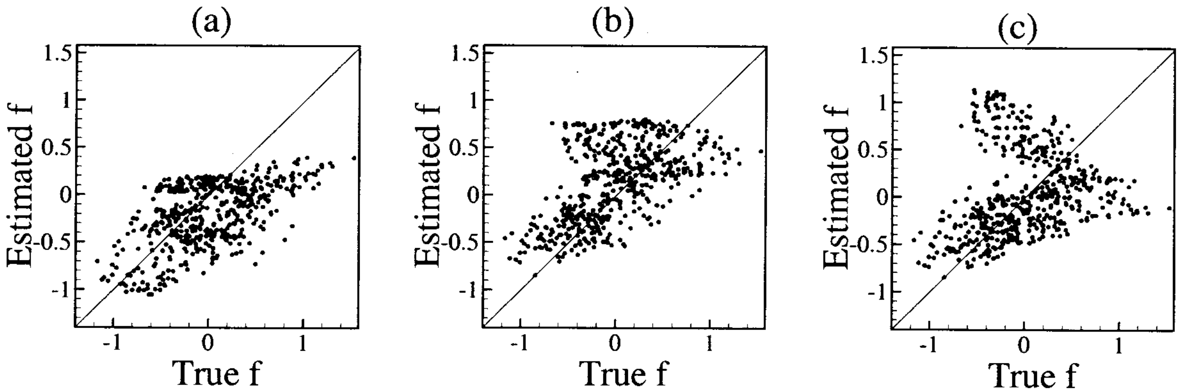

Figure 6. Scatterplot of true f versus estimated f using measurements of f and concentration for mean pressure heads of 30, -10, and -20, respectively.

tration variance becomes smaller and the nonlinearity between concentration and LnK_s is reduced. Furthermore, the cokriging covariance matrix becomes well behaved and does not require the addition of the measurement error term in the solution. While these factors improved our estimates of the conductivity field, the major improvement using the sequential approach over estimation using concentration measurements alone was due to the fact that more information was employed in the sequential estimation. The sequential estimate of f, shown in Figure 9, is only marginally superior to the estimate made by using head measurements. This indicates that concentration data are not very helpful in estimating hydraulic conductivity, using the cokriging technique.

Results of our analysis suggest that the arrival time information is useful for estimating f. Because arrival time is an integrated measurement (the integration of concentration over a time period), the nonlinear relationship between arrival time and LnK_s may be less than that between concentration and LnK_s. No stabilizing terms were necessary in the cokriging estimate when using arrival time. Nevertheless, arrival time, like concentration, is not as effective as head for the estimation of conductivity. This result appears to contradict the finding by *Harvey and Gorelick* [1995]. They showed that when sampling locations are separated over a distance of many correlation scales of conductivity, arrival time data provide better estimate than head data due to the long cross-correlation distance between arrival time and conductivity. The sampling locations in our case, however, were separated within one conductivity integral scale. This may explain the reason why the advantage of the long cross-correlation distance between arrival time and conductivity did not emerge in our analysis.

We must emphasize that our assessment of the different types of the secondary information is based on a linear estimator. It may not hold for a nonlinear estimator (e.g., successive linear estimator by *Yeh et al.* [1996] and *Zhang and Yeh* [1997]). Nevertheless, for real-world problems, it is clear that the ergodicity assumption cannot be easily satisfied for the solute transport case. Only when a plume has traveled over enough correlation lengths, sampled enough heterogeneity, and become well-mixed, will the ergodicity assumption be satisfied. At that time, the plume may encounter heterogeneity of different scales and the ergodicity will, thus, never be attained. Unless a nonlinear estimator is developed, the problems associated with how ergodicity impacts the nonlinear estimator remain unknown.

In addition to the difficulties associated with the use of concentration measurements to estimate conductivity in our hypothetical porous media, the exact location and strength of

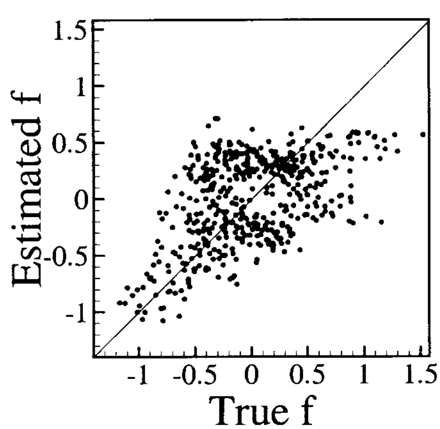

Figure 7. Scatterplot of true f versus estimated f using f and arrival times for the mean head 30 cm.

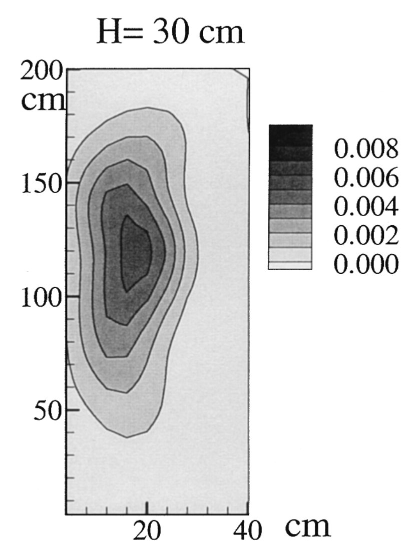

Figure 8. Conditional mean concentration distribution based on measurements of head and conductivity.

the solute source and the dispersivity must be acquired beforehand in any real-world problems. This problem also applies to the case where the arrival time is used. One must also recognize that head data are the easiest to collect in a field among the three types of data evaluated in this paper. The cost of collecting head information is also much lower than that of sampling concentration or arrival time. Exhaustive computational effort required for calculating sensitivity matrices and covariances is also another disadvantage if concentration and travel time measurements are used for estimating the hydraulic conductivity field. It takes a large amount of CPU time to calculate the sensitivity of arrival time because the calculation must continue until a complete breakthrough of the solute plume is observed at the sampling locations. In addition to the difficulties mentioned above, concentration information is also prone to large errors in sampling procedures. As a consequence, solute concentration and arrival time data may not be as useful in practices, although they provide useful information in theoretical analyses.

We showed that the assumption of ergodicity can be relaxed by the sequential approach. The sequential approach proves to be an efficient way to conduct cokriging when more than one type of data is available. The size of the cokriging matrix is significantly reduced when different data sets are used one after another. As a result, tremendous CPU time and computer memory can be saved, and the condition of the cokriging matrix is improved because of the reduction in its size. More importantly, the sequential algorithm increases the effectiveness of concentration measurements in estimating conductivity by providing a conditional mean concentration field, which relaxes the ergodicity assumption.

The result of the sequential estimation will depend on the sequence these data sets are applied. For instance, if the concentration measurements were used to estimate conductivity prior to the use of head data, the final estimated conductivity field would be different from that in Figure 9. This difference can be explained by the lack of linearity among these data sets. Not only the result would be different, but also the estimation would not be less accurate because concentration measurements cannot provide a better conditioning mean field due to the lack of ergodicity and linearity.

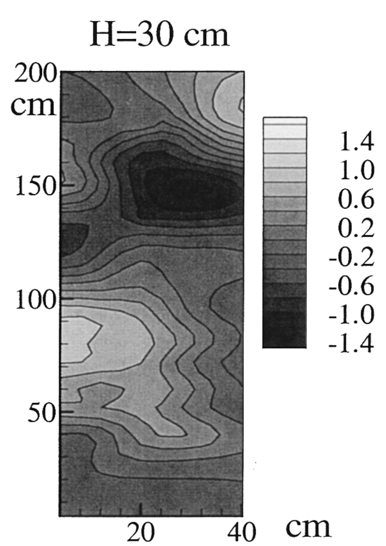

Figure 9. Estimated f field using f, head, and concentration measurements with the sequential approach.

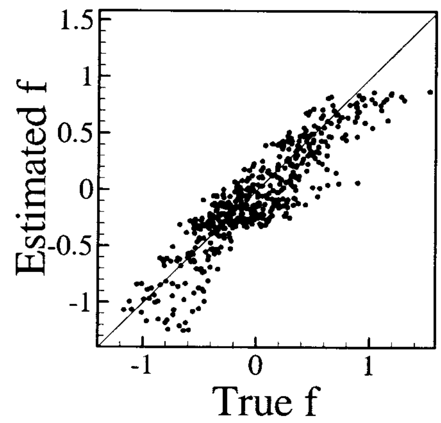

Figure 10. Scatterplot of true f versus estimated f using the sequential approach.

5. Conclusion

On the basis of our analysis, we conclude that the performance of cokriging based on either head or concentration measurements deteriorates as the medium becomes less saturated. This phenomenon is attributed to the increase in nonlinearity between head or concentration and the conductivity as the medium becomes less saturated.

The head measurements of steady state flow fields were found to be the most useful secondary information for the estimation of the LnK_s field, using the cokriging technique. This can be attributed to several factors. First, the nonlinear relationship between head and LnK_s may be mild in the cases studied. Additionally, the assumption of ergodicity is approximately satisfied for steady state flow. The existence of ergodicity reduces the variance of head and consequently improves the linearity between head and conductivity.

Conversely, the ergodicity assumption cannot be easily satisfied for the solute transport case. Only when a solute plume has traveled over enough correlation lengths, sampled enough heterogeneity, and become well mixed will the ergodicity assumption be satisfied. Because of the lack of ergodicity, the variance of concentration perturbation can be very large and the cokriging estimation using concentration measurements can be unsatisfactory.

We have developed a sequential approach that proves to be an efficient way to conduct cokriging when more than one type of data is available. More importantly, our approach relaxes the assumption of ergodicity in the situation where concentration measurements are used. Finally, we believe that our derivation of the adjoint state method derived here for flow and solute transport in variably saturated porous media is useful for developing different inverse or parameter estimation techniques. Although currently restricted to linear systems, our analysis is the first step toward the nonlinear conditioning of flow and solute transport in variably saturated porous media.

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