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Characterization of Aquifer Heterogeneity Using Transient Hydraulic Tomography

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Abstract

Hydraulic tomography is a cost-effective technique for characterizing the heterogeneity of hydraulic parameters in the subsurface. During hydraulic tomography surveys, a large number of hydraulic heads (i.e., aquifer responses) are collected from a series of pumping or injection tests in an aquifer. These responses are then used to interpret the spatial distribution of hydraulic parameters of the aquifer using inverse modeling. In this study, we developed an efficient sequential successive linear estimator (SSLE) for interpreting data from transient hydraulic tomography to estimate three-dimensional hydraulic conductivity and specific storage fields of aquifers. We first explored this estimator for transient hydraulic tomography in a hypothetical one-dimensional aquifer. Results show that during a pumping test, transient heads are highly correlated with specific storage at early time but with hydraulic conductivity at late time. Therefore, reliable estimates of both hydraulic conductivity and specific storage must exploit the head data at both early and late times. Our study also shows that the transient heads are highly correlated over time, implying only infrequent head measurements are needed during the estimation. Applying this sampling strategy to a well-posed problem, we show that our SSLE can produce accurate estimates of both hydraulic conductivity and specific storage fields. The benefit of hydraulic tomography for ill-posed problems is then demonstrated. Finally, to affirm the robustness of our SSLE approach, we apply the SSLE approach to transient hydraulic tomography in a hypothetical two-dimensional aquifer with nonstationary hydraulic properties, as well as a hypothetical three-dimensional heterogeneous aquifer.

Key words: *transient hydraulic tomography, SSLE, cokriging, temporal correlation, hydraulic conductivity, specific storage.*

1. Introduction

Detailed spatial distributions of hydraulic parameters are imperative to improve our ability to predict water and solute movement in the subsurface (e.g., Yeh, 1992, 1998). Traditional aquifer tests like pumping tests and slug tests only yield hydraulic parameters integrated over a large volume (e.g., Butler and Liu, 1993). Furthermore, the study by Wu et al. (2004) reports that the classical analysis for aquifer tests yields unrepresentative estimates of transmissivity and storage coefficient. For characterizing detailed spatial distributions of hydraulic parameters, a new method, hydraulic tomography (Gottlieb and Dietrich, 1995; Renshaw, 1996; Yeh and Liu, 2000; Liu et al., 2002; McDermott et al., 2003), which evolved from the CAT scan concept of medical sciences and geophysics, appears to be a viable technology.

Hydraulic tomography is, in the most simplified terms, a series of cross-well influence tests. In other words, an aquifer is stressed by pumping water from or injecting water into a well, and monitoring the aquifer's response at other wells. A set of stress/response yields an independent set of equations. Sequentially switching the pumping or injection location, without installing additional wells, results in a large number of aquifer responses caused by stresses at different locations and, in turn, a large number of independent sets of equations. This large number of sets of equations makes the inverse problem (i.e., using aquifer stress and response relation to estimate the spatial distribution of hydraulic parameters) better posed, and the subsequent estimate approaches reality.

Interpreting data from hydraulic tomography presents a challenge, however. The abundance of data generated during tomography can lead to information overload, and cause substantial computational burdens and numerical instabilities (Yeh, 1986, Hughson and Yeh, 2000). Moreover, the interpretation can be non-unique. Yeh and Liu (2000) developed a sequential successive linear estimator (SSLE) to overcome these difficulties. The SSLE approach eases the computational burdens by sequentially including information obtained from different pumping tests; it resolves the non-uniqueness issue by providing the best unbiased conditional mean estimate. That is, it conceptualizes hydraulic parameter fields as spatial stochastic processes and seeks their mean distributions conditioned on the information obtained from hydraulic tomography, as well as directly measured parameter values (such as from slug tests, or core samples). Using sand box experiments, Liu et al. (2002) demonstrated that the combination of hydraulic tomography and SSLE is a propitious, cost-effective technique for delineating heterogeneity using a limited number of invasive observations. The work by Yeh and Liu (2000), nonetheless, is limited to steady state flow conditions, which may occur only under special field conditions. Because of this restriction, their method ignores transient head data before flow reaches steady state conditions. Transient head data, although influenced by both hydraulic conductivity and specific storage, are less likely to be affected by uncertainty in boundary conditions. The development of a new estimation procedure thus becomes essential such that all datasets collected during hydraulic tomography surveys can be fully exploited.

Few researchers have investigated transient hydraulic tomography. For example, Bohling et al. (2002) exploited the steady-shape flow regime of transient flow data to interpret tomographic surveys. Under steady-shape conditions at late time of a pumping test before boundary effects take place, the hydraulic gradient changes little with time--a situation where sensitivity of head to the specific storage is small. As a consequence, the steady-shape method is useful for estimating hydraulic conductivity but not specific storage.

Their steady-shape method relies on the classical least-squares optimization method and the Levenberg-Marquardt algorithm (Marquardt, 1963) for controlling convergence issues (see Nowak and Cirpka, 2004). This optimization method is known to suffer from non-uniqueness of the solutions if the inverse problem is ill posed and regularization (Tikhonov and Arsenin, 1977) or prior covariance of parameters (Nowak and Cirpka, 2004) is not used. The least-squares approach is also computationally inefficient if every element in the solution domain (in particular, three-dimensional aquifers with multiple, randomly distributed parameters) is to be estimated. This inefficiency augments if the sensitivity matrices required by the optimization are not evaluated using an efficient algorithm, such as the adjoint state approach.

These shortcomings may be the reasons that test cases in Bohling et al. (2002) were restricted to unrealistic, perfectly stratified aquifers, where the heterogeneity has no angular variations, and specific storage is constant and known a priori. The assumption of a spatially constant and known specific storage value for the entire aquifer makes the inverse problem almost the same as the steady hydraulic tomography as explored by Yeh and Liu (2000). Perhaps the inverse problem of the transient tomography is less affected by unknown in boundary conditions. Lastly, for perfectly horizontal layered aquifers, many traditional hydraulic test methods, without resorting to hydraulic tomography, can easily estimate hydraulic properties of each layer using just one borehole.

Similar to Vasco et al. (2000), Brauchler et al. (2003) developed a method that uses the travel time of a pneumatic pressure pulse to estimate air diffusivity of fractured rock. Similar to X-ray tomography, their approach relies on the assumption that the pressure pulse travels along a straight line. Thus, an analytical solution can be derived for the propagation of the pressure pulse between a source and a pressure sensor. Many pairs of sources and sensors yield a system of one-dimensional analytical equations. A least-squares based inverse procedure developed for seismic tomography can then be applied to the system of equations to estimate the diffusivity distribution. The ray approach avoids complications involved in numerical formulation of the three-dimensional forward and inverse problems, but it ignores interaction between adjacent ray paths and possible boundary effects. Consequently, their method requires an extensive number of iterations and pairs of source/sensor data to achieve a comparable resolution to that achieved from inverting a three-dimensional model.

To our knowledge, no researchers have developed an inverse method for transient hydraulic tomography to estimate both hydraulic conductivity and specific storage of aquifers. For general groundwater inverse problems other than hydraulic tomography, Sun and Yeh (1992) assumed a specific storage field that was homogeneous and known a priori. They then developed a stochastic inverse method to estimate the spatial distribution of transmissivity using only transient head information. For transient hydraulic tomography, Vasco et al. (2000) and Brauchler et al. (2003) estimated diffusivity, the ratio of hydraulic conductivity to specific storage, without any attempt to separate the two parameters.

In this paper, we extended the SSLE developed by Yeh and Liu (2000) to transient hydraulic tomography for estimating randomly distributed hydraulic conductivity and specific storage in 3-D aquifers. This paper begins with the derivation of the SSLE for use with transient hydraulic heads. We introduce a loop iteration scheme to improve the accuracy of sequential usage of head data. We then verify our new approach by applying it to a synthetic one-dimensional heterogeneous aquifer. During this one-dimensional test, temporal variation of cross-correlation between transient heads and parameters, as well as temporal correlation of transient heads, is investigated. Results of this investigation lead to an effective sampling strategy, as opposed to developing an entire well hydraulic graph as used by Bohling et al. (2002), for efficient inversion of the transient hydraulic tomography data. To clarify the common myth about the stationary stochastic process assumption behind the SSLE approach (e.g., Kosugi and Inoue, 2002), we subsequently apply our new approach to a transient hydraulic tomographic survey in a hypothetical, two-dimensional nonstationary aquifer. Finally, the new SSLE is applied to a hypothetical three-dimensional, heterogeneous aquifer to demonstrate the robustness of our new approach.

2. Method

2.1 Groundwater Flow in Three-dimensional Saturated Media

In the following analysis, we assume that groundwater flow in three-dimensional, saturated, heterogeneous, porous media can be described by the following equation:

$$\nabla \cdot [K(\mathrm{x})\nabla H] + Q(x) = S_s(\mathrm{x})\frac{\partial H}{\partial t} \tag{1}$$

subject to boundary and initial conditions:

$$H\big|_{\Gamma_1} = H_1, \quad [K(\mathbf{x})\nabla H]\cdot \mathbf{n}\big|_{\Gamma_2} = q, \qquad \text{and } H\big|_{t=0} = H_0 \tag{2}$$

where in (1), H is total head (L), $\mathbf{x}$ is the spatial coordinate ($x = \{x_1, x_2, x_3\}$, (L), and x_3 represents the vertical coordinate and is positive upward), Q(x) is the pumping rate (1/T) at the location x, $K(\mathbf{x})$ is the saturated hydraulic conductivity (L/T), and $S_s(\mathbf{x})$ is the specific storage (L^{-1}). In equation (2), H_l is the prescribed total head at Dirichlet boundary Γ_1, q is the specific flux (L/T) at Neumann boundary Γ_2, $\mathbf{n}$ is a unit vector normal to the union of Γ_1 and Γ_2, and H_0 represents the initial total head. The equation is solved by a 3-D finite element approach developed by Srivastava and Yeh (1992) in the following analysis.

2.2 Sequential Successive Linear Estimator (SSLE)

The SSLE approach is an extension of the SLE (Successive Linear Estimator) approach (Yeh et al., 1996; Zhang and Yeh, 1997; Hanna and Yeh, 1998; Vargas-Guzman and Yeh, 1999, 2002; Hughson and Yeh, 2000). The SLE approach is essentially cokriging (Yeh et al., 1995)--Bayesian formalism (Kitanidis, 1986)--that seeks mean parameter fields conditioned on available point data as well as geological and hydrologic structures (i.e., spatial covariance functions of parameters and hydraulic heads, and their cross-covariance functions). Different from cokriging, SLE uses a linear estimator successively to update both conditional means and covariances such that the nonlinear relation between information and parameters is considered. As a stochastic estimator analogous to the direct method of the deterministic approach (see Yeh, 1986), SLE is different from the maximum a posterior (McLaughlin and Townley, 1996) and the quasi-linear geostatistical inverse approach (Kitanidis, 1995). The latter are merely least-squares optimization algorithms using the kriging or cokriging estimate as an initial guess and parameter covariances for regularization.

The SSLE approach relies on the SLE concept to sequentially include data sets and update covariances and cross-covariances in the estimation process. The sequential method avoids solving huge systems of equations and therefore reduces numerical difficulties. The approach has been successfully applied to parameter estimations in variably saturated media (e.g., Zhang and Yeh, 1997; Hanna and Yeh, 1998; Hughson and Yeh, 2000), steady hydraulic tomography (Yeh and Liu, 2000; Liu et al., 2002), electrical resistivity tomography (Yeh et al., 2002); and stochastic information fusion (Yeh and Šimůnek, 2002; Liu and Yeh, 2004). In this study, we extend this inverse approach to incorporate transient hydraulic head data to estimate both hydraulic conductivity and specific storage fields. As the majority of the SSLE method used in this study remains similar to that in previous works by Yeh and his colleagues, we present only a brief summary, but a sensitivity analysis for transient flow, and a new loop iteration scheme are given in detail below.

To characterize the heterogeneity of geological formations, the SSLE algorithm treats the natural logs of saturated hydraulic conductivity and specific storage as stochastic processes. We therefore assume $\ln K = \overline{K} + f$ and $\ln S_s = \overline{S} + s$, where $\overline{K}$ and $\overline{S}$ are mean values, and f and s denote the perturbations. The transient hydraulic head response to a pumping test in transient hydraulic tomography is represented by $H = \overline{H} + h$, where $\overline{H}$ is the mean and h is the perturbation. Substituting these stochastic variables into (1), taking the conditional expectation, and conditioning with some observations of head and parameters generates the mean flow equation as

$$\nabla\cdot[\bar{K}_{con}(\mathrm{x})\nabla\bar{H}_{con}]+Q=\bar{S}_{con}(\mathrm{x})\frac{\partial\bar{H}_{con}}{\partial t} \tag{3}$$

where $\bar{K}_{con}$, $\bar{H}_{con}$, and $\bar{S}_{con}$ are conditional effective hydraulic conductivity, hydraulic head and specific storage, respectively, and Q is the pumping rate at a given location, which is known a priori. Similar to the work by Yeh and his colleagues, we seek the conditional effect fields of hydraulic conductivity and specific storage, conditioned on the information from transient hydraulic tomography and some direct measurements of K and S_s.

The estimation procedure starts with a weighted linear combination of direct measurements of the parameters and transient head data at different locations to obtain the first estimate of the parameters. The weights are calculated based on statistical moments (namely, means, and covariances) of parameters, the covariances of heads, cross-covariances between heads and parameters, and cross-covariance of heads at different times. The first estimate is then used in the mean flow equation to calculate the head at observation locations and sampling times (i.e., forward simulation). Differences between the observed and simulated heads are determined subsequently. A weighted linear combination of these differences is then used to improve the previous estimates. Iterations between the forward simulation and estimation continue until the improvement in the estimates diminishes to a prescribed value.

a) Sensitivity analysis of transient flow

In the above estimation procedure, the head covariance in space and time and its cross-covariances with parameters are evaluated using a first-order approximation, which involves evaluation of sensitivity matrices of the governing flow equation. The sensitivity matrices are evaluated as follows. Transient hydraulic heads are expanded in a Taylor series around the mean values of parameters. After neglecting second and higher order terms, the transient hydraulic head is:

$$H = \overline{H} + f\frac{\partial H}{\partial f}\Big|_{\overline{K},\overline{H}} + s\frac{\partial H}{\partial s}\Big|_{\overline{S},\overline{H}} \qquad (4)$$

The sensitivity terms $\frac{\partial H}{\partial f}\Big|_{\overline{K},\overline{H}}$ and $\frac{\partial H}{\partial s}\Big|_{\overline{S},\overline{H}}$ in (4) are calculated by the adjoint state method (Sykes, et al. 1985; Li and Yeh, 1998). We briefly describe the method here (refer to Li and Yeh (1998, 1999), Sun and Yeh (1992) for a detailed derivation). The marginal sensitivity of a performance measure P to a parameter χ is defined as

$$\frac{dP}{d\chi} = \int_T \int_\Omega \left(\frac{\partial G}{\partial \chi} + \frac{\partial G}{\partial H}\frac{\partial H}{\partial \chi}\right) d\Omega dt \qquad (5)$$

where T and Ω represent time and spatial domain, respectively. The first term of the integral in (5) indicates the direct dependence of P on χ, while the second term indicates the implicit dependence of P on χ through the heads (Sykes et al., 1985). In this case,

$$G = H\delta(x - x_k)(t - t_l) \qquad (6)$$

representing the hydraulic head at location x_k and time t_l, where δ is Kronecker delta-function which equals unity if x equals x_k and t equals t_l, and equals zero otherwise.

Differentiating (1) with respect to a parameter χ, multiplying by a arbitrary function ϕ^*, integrating over T and Ω, applying Green's Identities, and dropping boundary terms gives

$$\int_T \int_\Omega \left[\frac{\partial S}{\partial \chi}\frac{\partial H}{\partial t}\phi^* + \frac{\partial K}{\partial \chi}\nabla H \nabla \phi^* - \phi S\frac{\partial \phi^*}{\partial t} - \phi\nabla\cdot(K\nabla\phi^*)\right] d\Omega dt + \int_\Omega S\phi^*\phi d\Omega\Big|_{t=0}^{t=T_e} = 0 \qquad (7)$$

where $\phi = \partial H/\partial\chi$ is the sensitivity of H to χ and is called state sensitivity, and T_e is the final simulation time. Adding (7) to the right hand side of (5), and substituting (6) for G, we have

$$\frac{dP}{d\chi} = \int_T \int_\Omega [\phi\delta(x - x_k)(t - t_l) + \frac{\partial S}{\partial\chi}\frac{\partial H}{\partial t}\phi^* + \frac{\partial K}{\partial\chi}\nabla H \nabla\phi^* - \phi S\frac{\partial\phi^*}{\partial t} - \phi\nabla\cdot(K\nabla\phi^*)]d\Omega dt$$
$$+ \int_\Omega S\phi^*\phi d\Omega\Big|_{t=0}^{t=T_e} \qquad (8)$$

We then choose the arbitrary function ϕ^* that satisfies

$$S\frac{\partial\phi^*}{\partial t} + \nabla\cdot(K\nabla\phi^*) - \delta(x - x_k)(t - t_l) = 0 \qquad (9)$$

with boundary and final conditions:

$$\phi^*\big|_{\Gamma_1} = 0, \qquad [K(\mathbf{x})\nabla\phi^*]\cdot\mathbf{n}\big|_{\Gamma_2} = 0, \qquad \phi^*\big|_{t=T_e} = 0 \qquad (10)$$

(note that (9) and (10) are called adjoint state equations); we further assume that the initial condition is known a priori, such that $\phi\big|_{t=0} = 0$, and hydraulic conductivity and specific storage are not correlated to each other. Thus, the sensitivities of the hydraulic head at location x_k and time t_l to f and s are given by

$$\frac{dH}{df_k} = \int_T\int_{\Omega_k}\left\{\frac{\partial K}{\partial f_k}\frac{\partial\phi^*}{\partial x_i}\frac{\partial H}{\partial x_i}\right\}dtd\Omega_k \qquad (11)$$

$$\frac{dH}{ds_k} = \int_T\int_{\Omega_k}\left\{\frac{\partial S}{\partial s_k}\phi^*\frac{\partial H}{\partial t}\right\}dtd\Omega_k \qquad (12)$$

where f_k and s_k are the perturbations of K and S at element k when the study domain is discretized. Note that the adjoint state equations are also transient problems and need to be solved backwardly in time. Also, the mean transient hydraulic heads must be derived beforehand in order to evaluate the sensitivities. The mean flow equation is given by equation (3). After ϕ^* and the mean head are calculated, the sensitivities obtained from equations (11) and (12) can be used to calculate covariances and cross-covariances.

b) Loop iteration scheme

As indicated by Vargas-Guzman and Yeh (2002) and Yeh and Šimůnek (2002) in previous SSLE approaches, the method of adding different data sets sequentially works best for linear systems. The relations between transient head and hydraulic parameters, however, are nonlinear; the sequential approach cannot fully exploit the head information. For instance, assume two datasets, A and B, are used in an inversion problem. The B dataset is added after the A dataset reaches convergence. The SSLE then stops after the B dataset converges. While the final estimates meet the convergence criteria for the B dataset, they may not now meet the convergence criteria for the A dataset. In addition, adding datasets in different sequences may lead to different results. Therefore, we introduced a new loop iteration scheme.

In this loop iteration scheme, the next dataset is added after all the datasets already incorporated meet the converge criteria within one loop. Specifically, a dataset is fed into SSLE first, and SSLE then iterates until this dataset meets a converge criterion. A new dataset is added afterwards, and SSLE again iterates until the new estimate convergences. Instead of adding the next new dataset, the scheme goes back to check the convergence for the first dataset. If the converge criterion is not met. The program starts a loop iteration in which the iteration involves both the first and second datasets. That is, the first dataset is iterated once, and then the second dataset is incorporated and iterated once also; we call this process a loop. The loop iteration continues until both datasets meet the converge criterion within one loop. Then, the next new dataset is added. The algorithm treats this new dataset similarly to the second dataset, except the loop iteration now involves three datasets. Additional datasets are added in a similar way. As a consequence, our inverse approach improves estimates throughout the loops, maximizes the usefulness of datasets, and alleviates the problems associated with the previous SSLE approach used by Yeh and his colleagues.

During a transient pumping test, one can record a large number of head observations at different times. As stated by Sun and Yeh (1992), simultaneous inclusion of transient head data at different times improves the estimates and decreases the head misfit because simultaneous inclusion considers the temporal correlation of transient heads. In our approach, we included in the estimation all observed heads at different times during a pumping activity. The head responses from different pumping tests are included sequentially.

3. Numerical Examples

3.1 One-Dimensional Flow

To test our inverse approach, a hypothetical, one-dimensional, horizontal, heterogeneous, confined aquifer was used. The aquifer was 20 meters long and was discretized into twenty elements. Each element was one meter long. The left and right sides of the aquifer were set as prescribed head conditions with hydraulic heads of 100m. Each element was assigned a hydraulic conductivity and a specific storage value using a stochastic random field generator (Gutjahr, 1989). The geometric mean of hydraulic conductivity was 0.225 m/d and the geometric mean of specific storage was 0.01 m^{-1}. The variance of lnK was 0.11 and the variance of lnS_s was 0.1.

Using this one-dimensional aquifer, a pumping test was simulated at location x = 9.5m with a pumping rate of 2.0 m^3/d. The flow approached a steady state condition after 16 days of pumping; about 95% of total drawdown occurred in the first 6 days of the pumping test. The cross correlation between head and parameters during the pumping test was then evaluated using a first-order analysis at five locations, x=1.5, x=3.5, x=5.5, x=7.5, and x= 9.5 m. Figure 1 depicts the behavior of cross correlation between h and f as a function of time at the five locations, and Figure 2 depicts the behavior of cross correlation between h and s. Each curve in the figures represents the cross correlation between head and parameter at the same location. Figure 1 shows that, in all locations, the cross correlation between h and f was low at early time and increased. Finally, it stabilized to a maximum value at a later time, around day seven. The cross correlation between h and s, however, increased sharply and reached its maximum value at an early time, only about two days, and then decreased and stabilized to its minimum value at a later time, around day thirteen (Figure 2). These results suggest that to obtain good estimates of f and s simultaneously, head information should be used that encompasses the entire pumping process -- including early time and late time.

The temporal correlation of transient heads was also evaluated. Figure 3 shows the contours of the temporal correlation of the head at x= 7.5 m from the beginning of the pumping test to 6 days. As indicated in the figure, the heads at different times were highly correlated, especially at later time. The high correlation suggests that the heads at a given observation location at different times provide overlapping information. In particular, the inclusion of heads at all time steps would be very computational time consuming for our estimator because the adjoint equations (9) and (10) must be solved once for each head observation in time. Because of the overlapping head information, choosing heads at several time steps instead of using heads at all time steps would significantly reduce the computation burdens and keep the usefulness of head information.

Based on the cross correlation and temporal correlation analysis, we thereafter tested our inverse approach for a well-posed inverse problem (deterministic inverse problems, Yeh et al., 1996). The head responses of all elements were collected at 0.5 days, 2.5 days, and 5.5 days, representing early, middle, and late times of the pumping test, respectively. One direct hydraulic conductivity measurement and one specific storage measurement were also assumed to be known at element one (i.e., the boundary fluxes are known). As a result, the necessary and sufficient conditions for inverse modeling (i.e., the transient head responses of all elements at two time steps, as well as boundary conditions) are fully specified, (see Sun, 1996 and Yeh and Šimůnek, 2002). The inverse problem thus becomes well posed and both parameter fields can be uniquely determined. Figures 4 and 5 compare the true hydraulic conductivity field and specific storage with estimates, respectively. The comparisons indicate that our new algorithm produces accurate estimates for both parameter fields for the deterministic case, and the accuracy of our SSLE method is ensured.

Next, we applied transient hydraulic tomography to the one-dimensional heterogeneous aquifer to demonstrate the benefit of a hydraulic tomography test. Four locations in the one dimensional aquifer were selected as pumping and observation wells. These four wells were located at x=3.5m, 7.5m, 11.5m, and 15.5m. The first pumping activity was initiated at x = 3.5m, and the corresponding head responses at all four wells were recorded. The pumping rate, pumping time, and observation times were the same as the pumping test of the previous deterministic case. The three additional pumping tests had the same configuration as the first one, except the pumping was initiated at x = 7.5m, x = 11.5 m, and x = 15.5 m for the second, third, and fourth pumping test, respectively. As a result, a total of 48 head responses were collected to estimate both parameters. Comparisons of the estimated hydraulic conductivity and specific storage with true parameters are shown in Figures 6 and 7, respectively. The two figures show that, with only four head observation locations out of a total of twenty elements of entire aquifer, the hydraulic tomography with our SSLE approach produces close estimates of the true spatial patterns for both parameters. As demonstrated in Figures 6a, b, c, and d, and Figure 7a, b, c, and d, the estimates progressively improved as more head responses from tomographic pumping tests were incorporated into our SSLE approach. However, the improvement of estimates from the third to the fourth pumping test was small, which indicates that excessive pumping tests only offer negligible estimate improvements for the given number of observation wells. These findings are similar to those reported by Yeh and Liu (2000).

3.2 Two-Dimensional Aquifer with Nonstationary Random Property Fields

A common myth about geostatistical or stochastic inverse methods is that they are limited by the stationary assumption (e.g., Kosugi and Inoue, 2002). To clarify such a misunderstanding, we applied our SSLE to hydraulic tomography in a synthetic nonstationary horizontal, confined aquifer. In this case, the parameters estimated in this case were transmissivity (*T*) and storage coefficient (*S*).

This aquifer was 15m long, and 15m wide and discretized into 225 elements; each element was 1m×1m. The left and right boundaries were assigned no-flow conditions while the other two sides and the initial condition were prescribed constant heads of 100m. Both the transmissivity and storage coefficient varied from element to element, but were constant within one element. Both parameters were generated as nonstationary random processes using the spectral method (Gutjahr, 1989). Specifically, the aquifer was divided into four zones and both parameters in each zone had a different mean and variance from other zones (Table 1), but all the zones had the same correlation scale of 5 meters in the x direction and 1 meter in the y direction. The detailed spatial distributions of both parameters are illustrated in Figures 8 and 9, respectively.

Nine wells (see Figure 8a for locations) were used for transient hydraulic tomography. Each pumping test lasted two days with a constant pumping rate of 1.0 m^3/d. The head data at 0.4 day, 1.2 days, and 2.0 days were collected at these wells. During the estimation process, the global geometric mean of the parameter fields of the entire aquifer, not the mean for each zone, were used as input. Further, we used correlation scales of 35 meters in the x direction and 5 meters in the y direction as our guess for the two parameter fields. Figure 8 and 9 show that our estimates clearly revealed the zonal structure of the aquifer and the details of heterogeneity within each zone. Therefore, our SSLE is not limited to stationary random fields—in fact, stationary or nonstationary is a subjective evaluation that varies according to the eye of the beholder.

3.3 Three-Dimensional Heterogeneous Aquifer

We subsequently applied our SSLE to transient hydraulic tomography in a synthetic three-dimensional heterogeneous confined aquifer. The geometry of this synthetic heterogeneous aquifer had dimensions of 15m × 15m × 15m, and was discretized into 3375 elements. Each element had a uniform size of 1m × 1m × 1m. The bottom and the top boundaries were set as no-flow, and the remaining four sides were assumed to be a prescribed hydraulic head of 100 m. A three-dimensional Cartesian coordinate system was used for spatial references. The coordinates of the bottom corner at the inner center of the cube (see Figure 10) were assigned to be (0, 0, 0) and the upper corner opposite to the bottom corner was assigned (15, 15, 15). The heterogeneous parameter fields again were generated by the spectral method (Gutjahr, 1989). The geometric mean of K was 0.34 m/d and the variance of ln$K$ was 0.5, while the geometric mean of S_s was 0.0002 m^{-1} and the variance of lnS_s was 0.1. The correlation scales in the x, y, and z directions were 20m, 20m, and 2m, respectively.

Four fully penetrating, multi-level wells were placed vertically in the aquifer. The horizontal coordinates for the four wells were (3.5, 3.5), (11.5, 3.5), (3.5, 11.5), and (11.5, 11.5). Each well had seven head observation ports whose vertical coordinates were 1.5 m, 3.5 m, 5.5 m, 7.5 m, 9.5 m, 11.5 m, and 13.5 m, respectively. Each well also had two pumping ports whose vertical coordinates were 4.5 m and 10.5 m, respectively. One direct hydraulic conductivity measurement and one specific storage measurement were assumed to be known at location (3.5, 3.5, 8.5). A pumping test was performed at one of the pumping ports with a constant pumping rate of 150 m^3/d. The pumping test was simulated for 0.01 day with a time step of 0.0005 day. The head responses at all 28 observation points were monitored at time 0.002 day, 0.006 day, and 0.01 day. Seven additional pumping tests were simulated, using the same pumping rate and pumping time period, but different pumping ports. A total of 672 head observations were used in our SSLE approach to simultaneously estimate hydraulic conductivity and specific storage.

The SSLE was implemented on a parallel computing platform using the LINUX operating system; the interpretation of the hydraulic tomography tests was carried out using a 10-node PC cluster (Pentium 4 2.8 GHz CPU each); the total computing time for the interpretation was 610 minutes.

Figures 10 a, b, c, and d plot the estimated hydraulic conductivity after two, four, six, and eight pumping tests, respectively, and the true hydraulic conductivity field is shown in Figure 10e. The estimated specific storage fields after two, four, six, and eight pumping tests are illustrated in Figures 11a, b, c, and d with the true field shown in Figure 11e. Both figures 10 and 11 demonstrate that the estimates from the first two pumping tests already have captured the general pattern of heterogeneity of the aquifer; the final estimates after eight pumping tests revealed greater details, although the improvement of the estimates decreased as more pumping tests were conducted.

Figure 12a is a scatterplot of true hydraulic conductivity values versus those estimated after eight pumping tests and Figure 12b is the scatterplot of true specific storage values versus estimated ones. According to these figures, our estimates were unbiased with some variance, which is expected since the inverse problem is not well posed (underdetermined). Notice that the axes of both figures are log scale. The results were also quantitatively evaluated using the average absolute error norm L1 and the mean-square error norm L2, defined as:

$$L1=\frac{1}{n}\sum_{i=1}^{n}\left|\hat{\chi}_i-\chi_i\right|,\quad L2=\frac{1}{n}\sum_{i=1}^{n}\left(\hat{\chi}_i-\chi_i\right)^2 \tag{12}$$

where $\hat{\chi}$ and χ are estimated and true parameters, respectively, and n is the number of elements. The changes of L1 and L2 with increasing number of pumping tests are shown in Figures 13a and b for hydraulic conductivity and specific storage, respectively. As more pumping tests were added, the values of L1 and L2 decreased, but the rate of reduction diminished. These results have the same trend as we found in the one-dimensional case.

Robust as they are, neither the hydraulic tomography nor our SSLE is a perfect method. The more head observations are collected, the higher the resolution of the estimates will be (i.e., there is no optimal). Inaccurate head observations and hydraulic property measurements (i.e., noises) during hydraulic tomography unequivocally can lead to an inaccurate estimate or stability of the estimate. While our SSLE can overcome the impacts of noise, the estimates become smooth, which means there is a loss of effectiveness of information. These issues have been discussed in Yeh and Liu (2000).

4 Conclusions

The three synthetic cases show that transient hydraulic tomography is a promising and viable tool for detecting detailed spatial variations of hydraulic parameters with a limited number of wells. Our SSLE can provide unbiased estimates of multiple parameters simultaneously, and reveal their detailed spatial distributions for both stationary and nonstationary random hydraulic property fields. In addition, our SSLE permits sequential inclusion of head data from different pumping tests, such that the size of the covariance matrix is small and can be solved with relative ease. By using a loop-iteration scheme, our new SSLE improves estimates throughout the loops and maximizes the usefulness of head information.

The cross-covariance analysis reveals that the cross correlation between head and hydraulic parameters varies temporally during a pumping test. The cross correlation between head and specific storage is high at early time, while the cross correlation between head and hydraulic conductivity is high at a later time because of constant head boundary conditions that facilitate steady flow. To simultaneously estimate hydraulic conductivity and specific storage parameters, the head information used in the inverse modeling needs to include both early and late times.

The transient heads are highly temporally correlated, especially at later times. Such a temporal correlation structure allows our SSLE to use only a few selected heads at some time steps, instead of all available heads at all time steps, to reduce computational cost, while keeping the usefulness of the head information.

Our SSLE approach involves backward calculation of adjoint equations during the sensitivity analysis for transient flow. For the same number of observation locations, a transient pumping test generates much more head information than a steady state pumping test. Even when head data are used for only a few selected time steps, instead of all time steps, the computational burden of transient hydraulic conductivity is significantly greater than steady state hydraulic tomography. Our SSLE approach is implemented on a parallel platform to ease the computational burden, such that the simulation time is reduced.

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Table 1: Statistical properties of the nonstationary aquifer

	Geometric mean of transmissivity (m^2/d)	Variance of ln transmissivity	Geometric mean of Storage coefficient	Variance of ln Storage coefficient
zone 1	0.250	0.150	0.001	0.040
zone 2	0.030	0.110	0.008	0.080
zone 3	0.320	0.121	0.002	0.009
zone 4	0.040	0.120	0.007	0.060

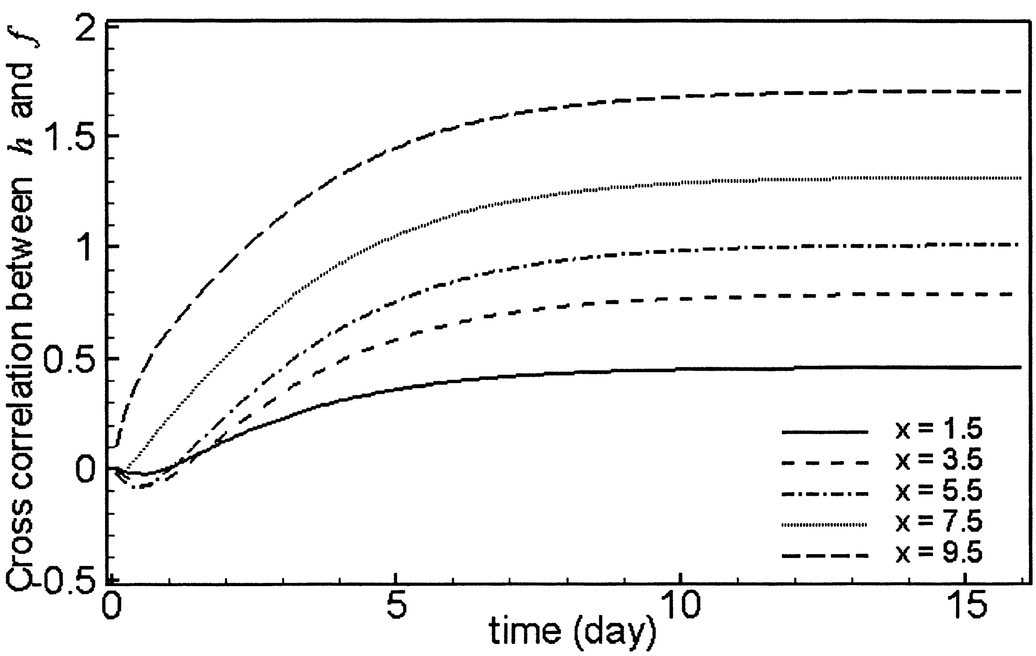

Figure 1. Cross correlation between h and f as a function of time during a pumping test.

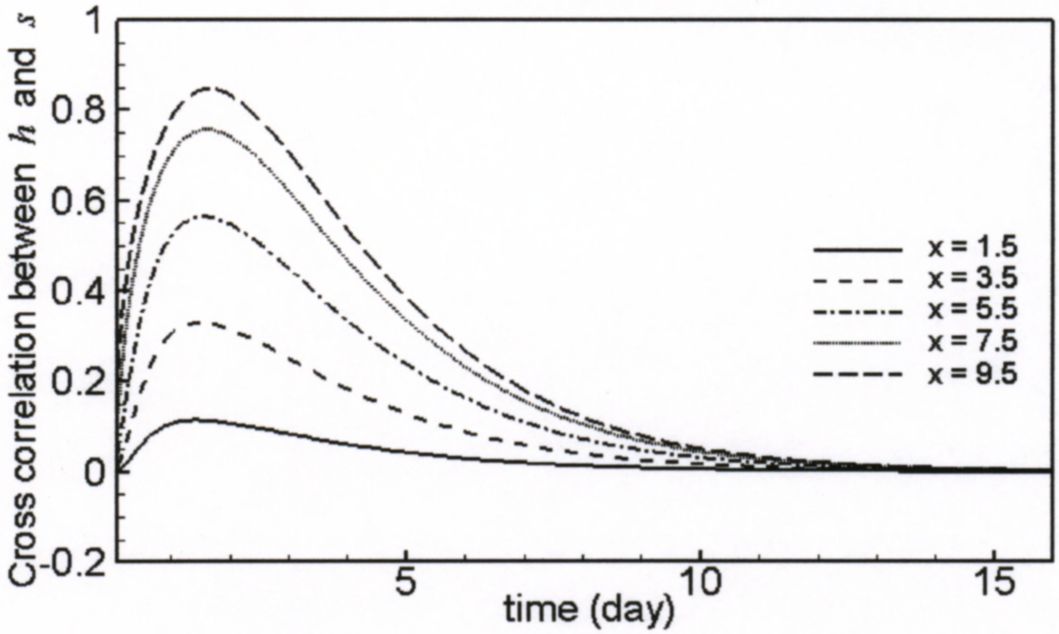

Figure 2. Cross correlation between h and s as a function of time during a pumping test.

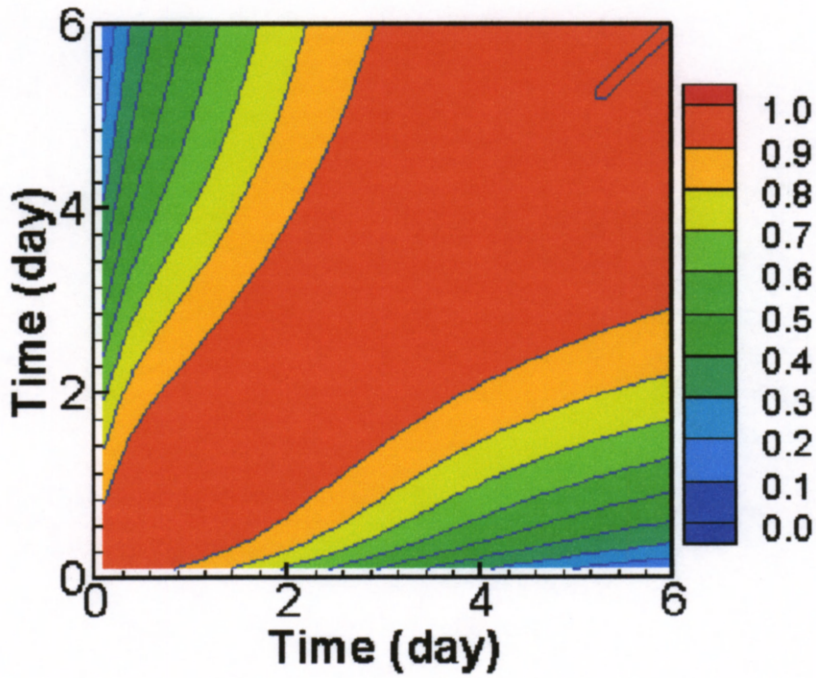

Figure 3. Temporal correlation of transient heads at x =7.5 m during a pumping test.

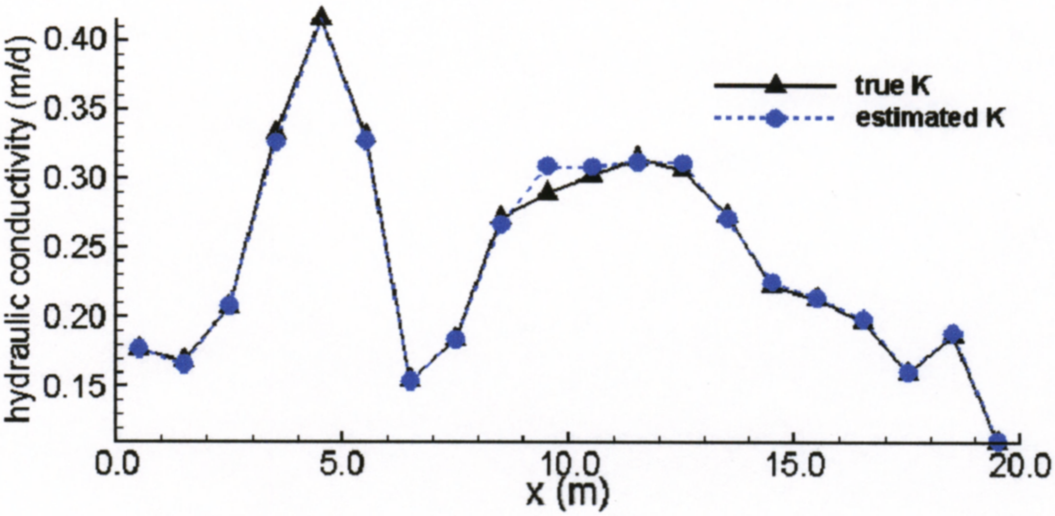

Figure 4. Comparison of estimated hydraulic conductivity with true hydraulic conductivity in a deterministic case.

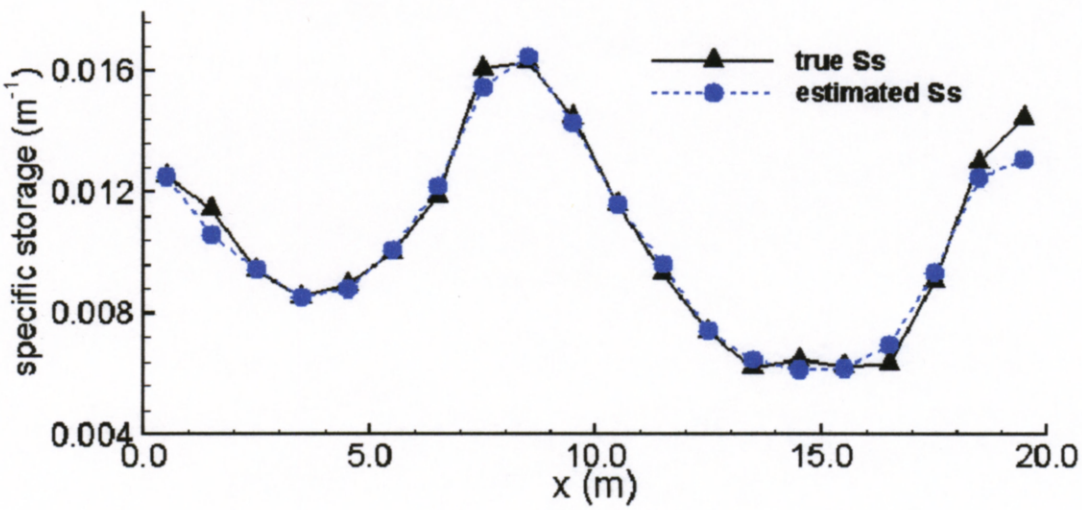

Figure 5. Comparison of estimated specific storage with true specific storage in a deterministic case.

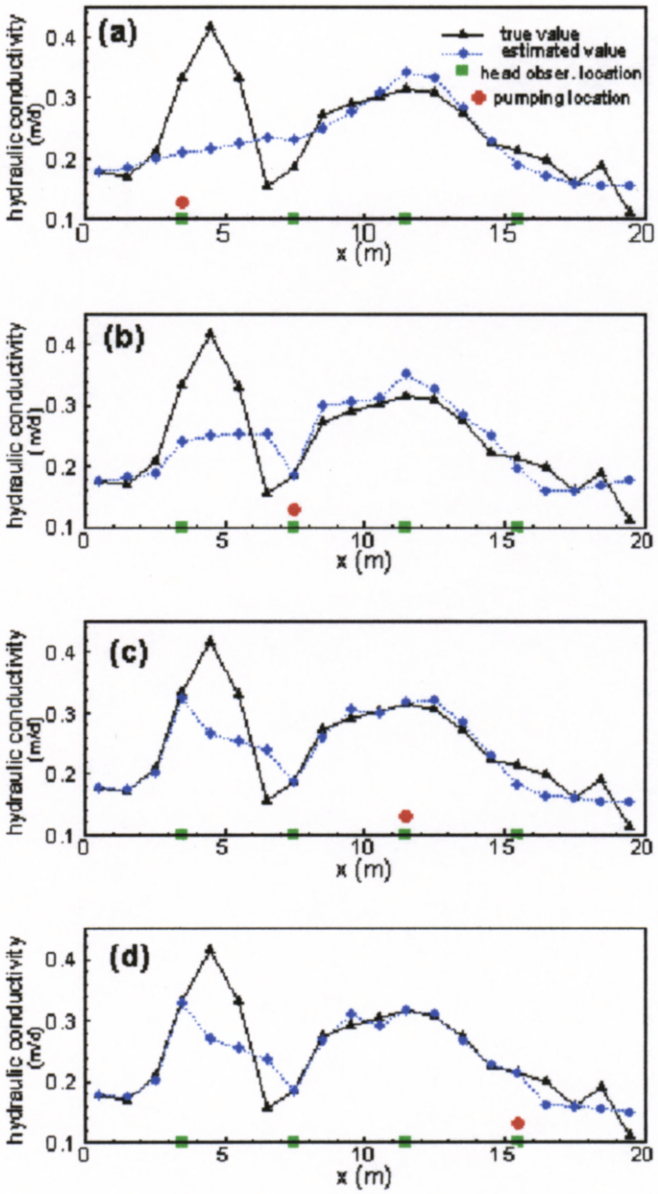

Figure 6 Estimated hydraulic conductivity from transient hydraulic tomography (a) estimates from the first pumping test; (b) estimates from the additional second pumping test; (c) estimates from the additional third pumping tests; (d) estimates from the four pumping tests.

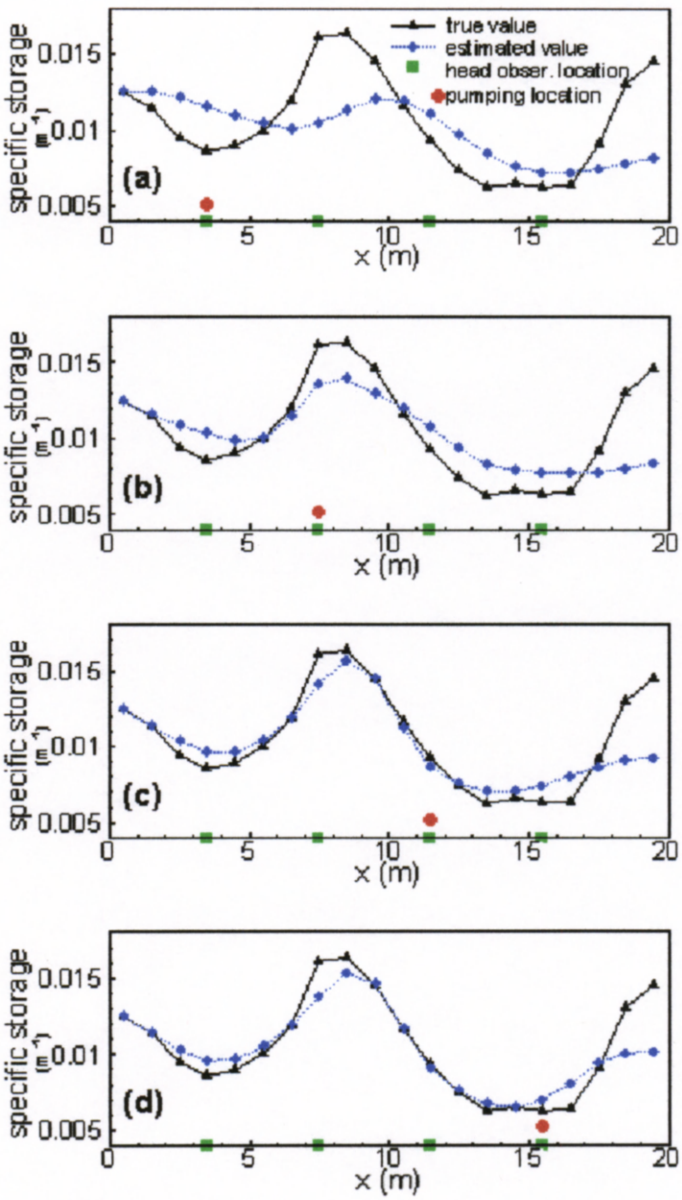

Figure 7 Estimated specific storage from transient hydraulic tomography (a) estimates from the first pumping test; (b) estimates from the additional second pumping tests; (c) estimates from the additional third pumping tests; (d) estimates from the fourth pumping tests.

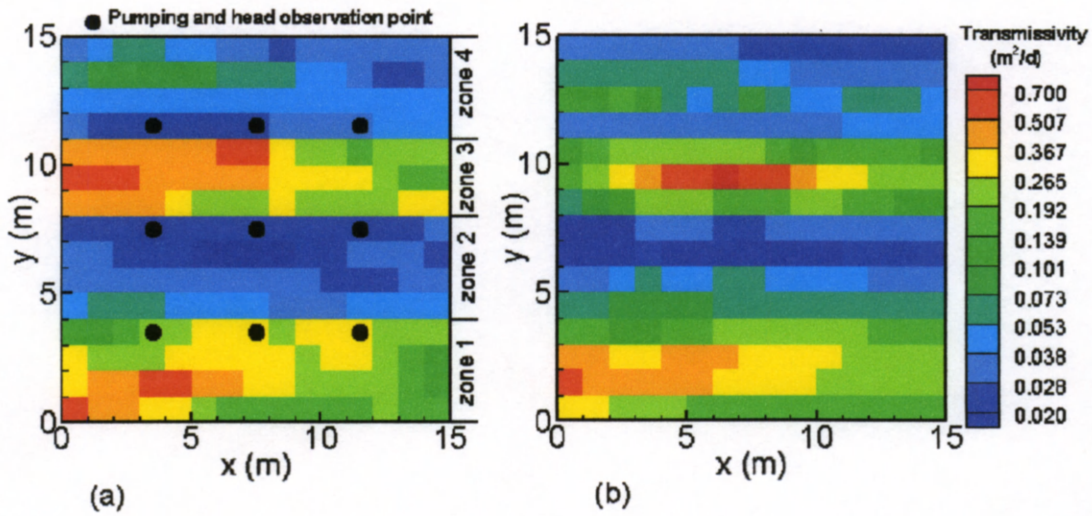

Figure 8 Comparison between (a) true transmissivity field and (b) estimated transmissivity field for a 2-D aquifer with nonstationary hydraulic properties.

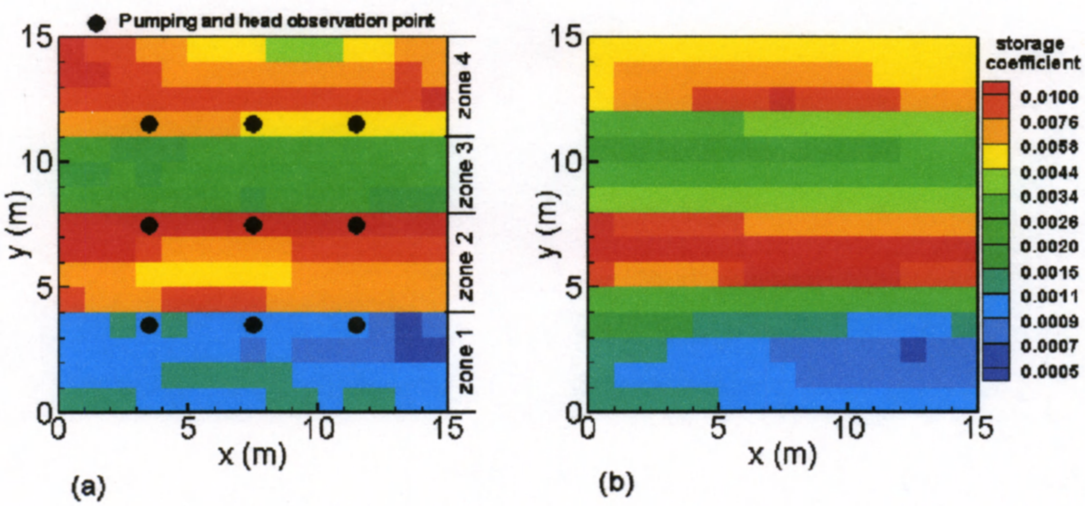

Figure 9 Comparison between (a) true storage coefficient field and (b) estimated storage coefficient field for a 2-D aquifer with nonstationary hydraulic properties.

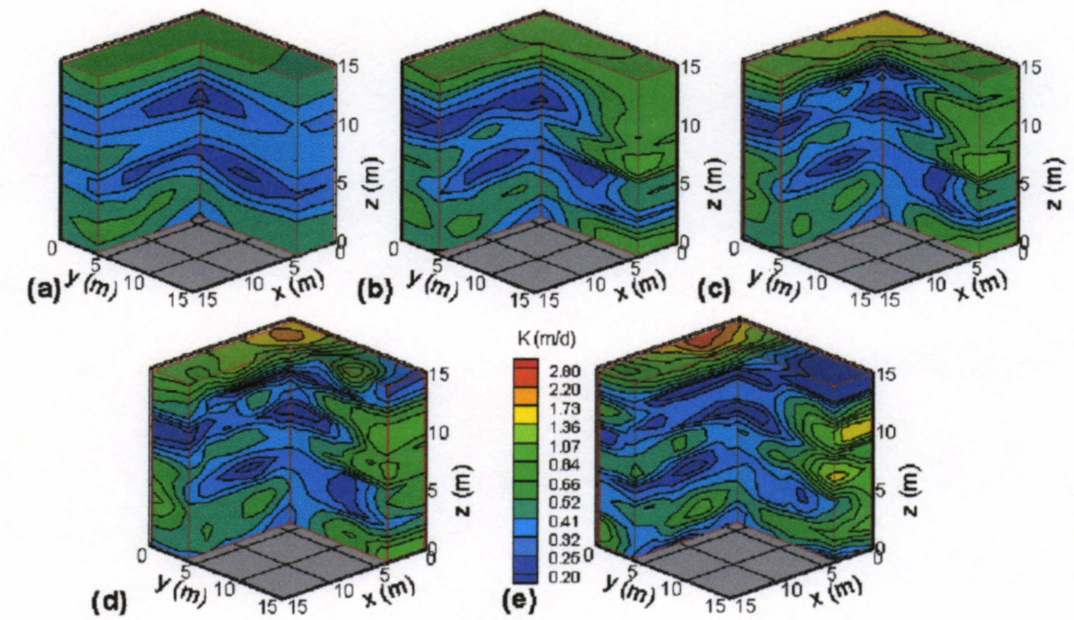

Figure 10 Comparison between estimated hydraulic conductivity with the true field in a three dimensional aquifer: estimated hydraulic conductivity field after (a) two, (b) four, (c) six, (d) and eight pumping tests, and (e) the synthetic true hydraulic conductivity field.

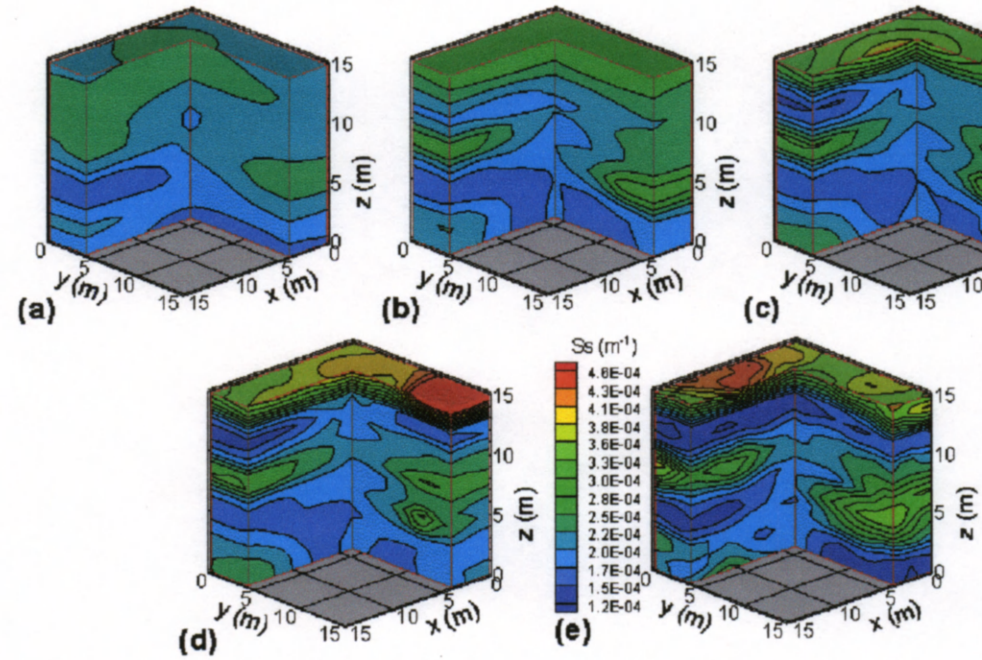

Figure 11. Comparison between estimated specific storage with the true field in a three dimensional aquifer: estimated specific storage field after (a) two, (b) four, (c) six, (d) and eight pumping tests, and (e) the synthetic true hydraulic conductivity field.

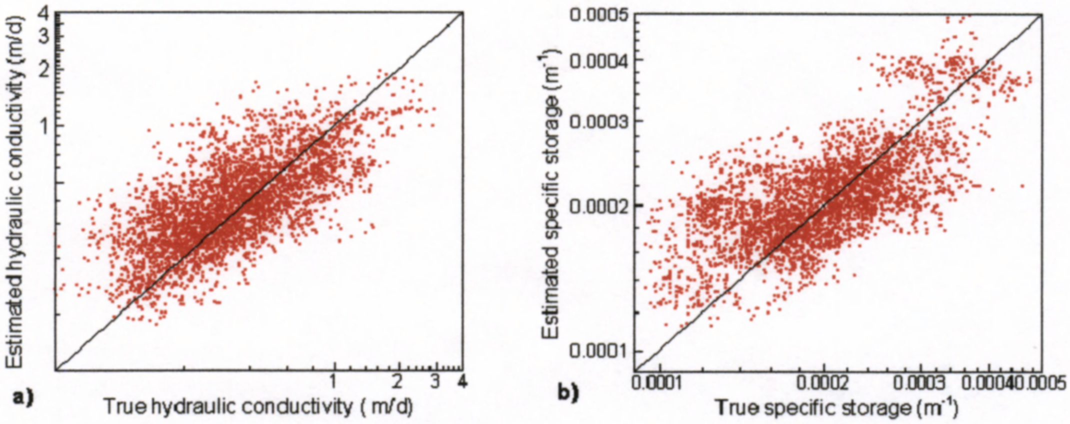

Figure 12. Scatterplots of a) estimated vs. true hydraulic conductivity; b) estimated vs. true specific storage.

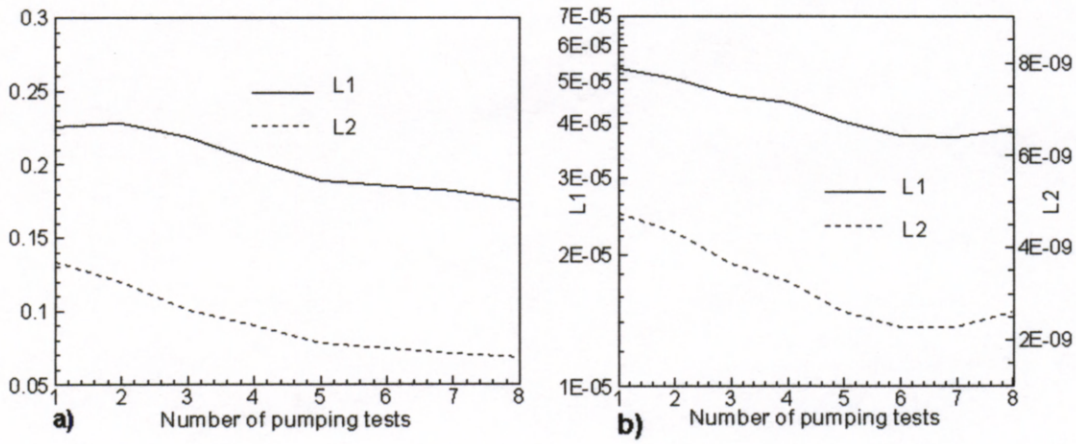

Figure 13. Statistical norms of our estimates: a) hydraulic conductivity; b) specific storage.