Characterization of aquifer heterogeneity using transient hydraulic tomography

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[1] 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 threedimensional hydraulic conductivity and specific storage fields of aquifers. We first explored this estimator for transient hydraulic tomography in a hypothetical onedimensional 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 a hypothetical three-dimensional heterogeneous aquifer.

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1. Introduction

[2] 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 of geologic media [e.g., Butler and Liu, 1993; Beckie and Harvey, 2002]. On the other hand, Wu et al. [2005] reported that the classical analysis for aquifer tests yields spurious transmissivity estimates and storage coefficient estimates that reflect local geology. 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 (computerized axial tomography) scan concept of medical sciences and geophysics, appears to be a viable technology.

[3] Hydraulic tomography is, in the most simplified terms, a series of cross-well interference 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

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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.

[4] 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 nonunique. *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 nonuniqueness 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 so that all data sets collected during hydraulic tomography surveys can be fully exploited.

[5] Few researchers have investigated transient hydraulic tomography. 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.

[6] 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 nonuniqueness 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, threedimensional 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.

[7] These shortcomings may be the reasons that test cases of 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 inversion of the transient tomography by Bohling et al. [2002] is less affected by unknown in boundary conditions. Nonetheless, 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.

[8] 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 rocks. Similar to X-ray tomography, their approach relies on the assumption that the pressure pulse travels along a straight line or a curve path. 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. Vesselinov et al. [2001] applied an optimization technique and geostatistics to pneumatic cross-borehole tests in fractured rocks. Because of the baseline of the pneumatic properties is unknown, it is difficult to assess the accuracy of their results.

[9] To our knowledge, few 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.

[10] 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 a better understanding of effects of conditioning using head measurements on estimates of hydraulic conductivity and specific storage, and an effective sampling strategy, as opposed to utilizing an entire drawdown time history, for efficient inversion of the transient hydraulic tomography data. 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

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

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

subject to boundary and initial conditions:

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

where in equation (1), H is total head (L), \bf{x} is the spatial coordinate $(x = {x_1, x_2, x_3}, (L)$, and x_3 represents the vertical coordinate and is positive upward), $Q(\mathbf{x}_n)$ is the pumping rate (1/T) at the location x_p , $K(x)$ is the saturated hydraulic conductivity (L/T), and $S_s(x)$ is the specific storage (L^{-1}) . In equation (2), H_1 is the prescribed total head at Dirichlet boundary Γ_1 , q is the specific flux (L/T) at Neumann boundary Γ_2 , **n** is a unit vector normal to the union of Γ_1 and Γ_2 , and H_0 represents the initial total head. The equations are solved by a 3-D finite element approach developed by Srivastava and Yeh [1992] in the following analysis.

2.2. Sequential Successive Linear Estimator

[12] The SSLE approach is an extension of the SLE (successive linear estimator) approach [Yeh et al., 1996; Yeh and Zhang, 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 geologic 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 based on differences between observed and simulated hydraulic heads successively to update both conditional means and covariances of the estimates such that the nonlinear relation between information and parameters is considered. As a stochastic estimator analogous to the direct method of the deterministic approach [Yeh, 1986], SLE is conceptually the same as but methodologically different from the maximum a posterior [McLaughlin and Townley, 1996] and the quasi-linear geostatistical inverse approach [Kitanidis, 1995].

[13] 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 Simunek, 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 our previous works, we present only a brief summary, but a sensitivity analysis for transient flow, and a new loop iteration scheme are given in detail below.

[14] To characterize the heterogeneity of geologic 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

$$
\nabla \cdot \left[\overline{K}_{con}(\mathbf{x}) \nabla \overline{H}_{con} \right] + \mathcal{Q}(\mathbf{x}_p) = \overline{S}_{con}(\mathbf{x}) \frac{\partial H_{con}}{\partial t}
$$
(3)

where \overline{K}_{con} , \overline{H}_{con} , and \overline{S}_{con} are conditional effective hydraulic conductivity, hydraulic head and specific storage, respectively [Yeh et al., 1996]. Similar to our previous work, we seek the conditional effective fields of hydraulic conductivity and specific storage, conditioned on the information from transient hydraulic tomography and some direct measurements of K and S_s .

[15] 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 in space and time, the cross covariances between heads and parameters. The first estimate is then used in the mean flow equation (3) to calculate the heads 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. 2.2.1. Sensitivity Analysis of Transient Flow

[16] 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 about the mean values of parameters. After neglecting second- and higher-order terms, the transient hydraulic head is

$$
H(\mathbf{x},t) = \overline{H}(\mathbf{x},t) + f(\mathbf{x}) \frac{\partial H(\mathbf{x},t)}{\partial \ln K(\mathbf{x})} \Big| \overline{\kappa} \overline{s} + s(\mathbf{x}) \frac{\partial H(\mathbf{x},t)}{\partial \ln S_{s}(\mathbf{x})} \Big| \overline{\kappa} \overline{s} \quad (4)
$$

The sensitivity terms $\frac{\partial H}{\partial \ln K}\Big|_{\overline{K},\overline{S}}$ $\left| \overline{\kappa}, \overline{s} \right|$ and $\frac{\partial H}{\partial \ln S_s} \left| \overline{\kappa}, \overline{s} \right|$ $\left|_{\overline{K},\overline{S}}\right|$ in equation (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

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

where T and Ω represent time and spatial domain, respectively. The first term of the integral in equation (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,

$$
G = H\delta(x - x_k)(t - t_l) \tag{6}
$$

representing the hydraulic head at location x_k and time t_l , where δ is Kronecker delta function which equals unity if

Figure 1. Cross correlation between h at $x = 9.5$ m and f at different locations for three selected times during a pumping test.

x equals x_k and t equals t_l , and equals zero otherwise. We choose an arbitrary function ϕ^* that satisfies

$$
S\frac{\partial \phi^*}{\partial t} + \nabla \cdot (K\nabla \phi^*) - \delta(x - x_k)(t - t_l) = 0 \tag{7}
$$

with boundary and final conditions:

$$
\phi^*|_{\Gamma_1} = 0, \quad [K(\mathbf{x}) \nabla \phi^*] \cdot \mathbf{n}|_{\Gamma_2} = 0, \quad \phi^*|_{t = T_e} = 0 \tag{8}
$$

(note that equations (7) and (8) are called adjoint state equations); we further assume that the initial condition is known a priori, such that $\phi|_{t=0} = 0$, 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 at location x_n are given by

$$
\frac{\partial H(\mathbf{x}_k, t_l)}{\partial \ln K(\mathbf{x}_n)} = \int\limits_T \int\limits_\Omega \left\{ \frac{\partial K(\mathbf{x})}{\partial \ln K(\mathbf{x}_n)} \frac{\partial \varphi^*}{\partial x_i} \frac{\partial H}{\partial x_i} \right\} dt d\Omega \tag{9}
$$

$$
\frac{\partial H(\mathbf{x}_k, t_l)}{\partial \ln S_s(\mathbf{x}_n)} = \int\limits_T \int\limits_\Omega \left\{ \frac{\partial S(\mathbf{x})}{\partial \ln S_s(\mathbf{x}_n)} \phi^* \frac{\partial H}{\partial t} \right\} dt d\Omega \tag{10}
$$

where $\ln K(\mathbf{x}_n)$ and $\ln S_s(\mathbf{x}_n)$ are the $\ln K$ and $\ln S_s$ at element n, respectively, 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 (9) and (10) can be used to calculate head covariances and its cross covariances with parameters, using a first-order approximation [Hughson] and Yeh, 2000].

2.2.2. Loop Iteration Scheme

[17] As indicated by Vargas-Guzman and Yeh [2002] and Yeh and Simunek [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 data sets, A and B, are used in an inversion problem. The B data set is added after the A data set reaches convergence. The SSLE then stops after the B data set converges. While the final estimates meet the convergence criteria for the B data set, they may not now meet the convergence criteria for the A data set. In addition, adding data sets in different sequences may lead to different results. Therefore we introduced a new loop iteration scheme.

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

[19] 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

Figure 2. Cross correlation between h at $x = 9.5$ m and s at different locations for three selected times during a pumping test.

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

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 some selected 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

[20] To test our inverse approach, a hypothetical, onedimensional, horizontal, heterogeneous, confined aquifer was used. The aquifer was 20 m long and was discretized into twenty elements. Each element was 1 m long. The left and right sides of the aquifer were set as prescribed head conditions with hydraulic heads of 100 m. Each element was assigned a hydraulic conductivity value and a specific storage value using a stochastic random field generator [Gutjahr, 1989]. The geometric mean of hydraulic conductivity was 0.0026 m/s and the geometric mean of specific storage was 0.0001 m^{-1} . The variance of lnK was 0.5 and the variance of $\ln S$ _s was 0.2. The correlation scales

Figure 4. Estimated and true hydraulic conductivity fields in the 1-D deterministic case.

Figure 5. Estimated with true specific storage fields in the 1-D deterministic case.

for both parameters are 5 m and $\ln K$ and $\ln S_s$ are assumed to be independent from each other, representing the worst scenario.

[21] Using this one-dimensional aquifer, a pumping test was simulated at location $x = 9.5$ m with a pumping rate of 0.005 m³/s. The flow approached a steady state condition after 19 s of pumping; about 95% of total drawdown occurred in the first 8 s of the pumping test. The cross correlation between head and parameters during the pumping test was evaluated using a first-order approximation and then examined. Figure 1 depicts behaviors of the cross correlation between observed h at $x = 9.5$ m and f at different locations in the aquifer at three selected times (2, 4, and 6 s). Likewise, Figure 2 depicts behaviors of the cross correlation between h and s at the three times. The cross correlation between h and f generally decreased with the distance away from the head observation location ($x =$ 9.5 m) but the cross correlation over the entire aquifer increased with time. Also, the number of f values having significant cross correlation (say, cross correlation values greater than 0.4) with the head at the observation location increased. Shapes of the cross-correlation functions are different from those in uniform flow [Mizell et al., 1980] due to converging flow and boundary conditions. Under uniform flow conditions, a head is negatively correlated with the hydraulic conductivity values down gradient and positively correlated with the hydraulic conductivity up gradient. Figure 2 shows that the cross correlation between the h and the s field decreased with time. At early time, strong cross correlations between h and s are confined to the vicinity of the observed head location. These cross correlations, nevertheless, dropped drastically at late time. Such results suggest that a head measurement in a well at late time can provide good estimates of f over a large portion of the aquifer. On the other hand, head measurements in a well can only yield information of the s nearby and only early time data are useful for the estimate of s. This finding supports the conclusion by Wu et al. [2005] that the storage coefficient estimate from a traditional aquifer test based on the drawdown time data in an observation well, induced by pumping at another well, is dominated by the local geology between the pumping well and the observation well. Furthermore, to obtain good estimates of f and s during hydraulic tomography tests, head information, encompassing the entire pumping process, including early time and late time, should be used. The resolution of the estimated f field will be better than that of the s field because of the localized influence of a head measurement on the estimate of s field.

Figure 6. Estimated hydraulic conductivity field from transient hydraulic tomography from (a) the first pumping test, (b) inclusion of the second test, (c) the third test, and (d) the fourth tests.

[22] 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 8 s. As indicated in Figure 3, 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, inclusion of heads at all time steps would be very computational time consuming for our estimator because the adjoint equations (7) and (8) 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.

[23] On the basis of 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 2, 4, and 6 s, 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 20 (i.e., the boundary fluxes are known). Therefore 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 [Sun, 1994; Yeh and Simunek, 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 thus ensured.

Figure 7. Estimated specific storage field from transient hydraulic tomography from (a) the first pumping test, (b) inclusion of the second test, (c) the third test, and (d) the fourth tests.

Figure 8. Estimated hydraulic conductivity field after (a) two, (b) four, (c) six, and (d) eight pumping tests and (e) the synthetic true hydraulic conductivity field of the 3-D aquifer.

[24] Next, we applied transient hydraulic tomography to the one-dimensional heterogeneous aquifer to demonstrate the benefit of a transient hydraulic tomography test. Four locations in the one dimensional aquifer were selected as pumping and observation wells. These four wells were located at $x = 3.5$ m, 7.5 m, 11.5 m, and 15.5 m. The first pumping activity was initiated at $x = 3.5$ m, 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 $x = 7.5$ m, $x = 11.5$ 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

Figure 9. Estimated specific storage field after (a) two, (b) four, (c) six, and (d) eight pumping tests and (e) the synthetic true specific storage field of the 3-D aquifer.

Figure 10. Frequency distributions of estimation errors: (a) hydraulic conductivity field and (b) specific storage field of the 3-D aquifer.

hydraulic conductivity and specific storage with true parameters are shown in Figures 6 and 7, respectively. Figures 6 and 7 show that with only four head observation locations out of a total of 20 elements of the 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, 6b, 6c, 6d, 7a, 7b, 7c, and 7d, 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 improvements for the given number of observation wells. These findings are similar to those reported by Yeh and Liu [2000].

3.2. Three-Dimensional Heterogeneous Aquifer

[25] 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 15 m \times 15 m \times 15 m, and was discretized into 3375 elements. Each element had a uniform size of 1 m \times 1 m \times 1 m. 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 8) were assigned to be (0, 0, 0) and the upper corner opposite to the bottom corner was assigned to be (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 $\ln S_s$ was 0.1. The correlation scales in the x, y, and z directions were 20 m, 20 m, and 2 m, respectively.

[26] Four fully penetrating, multilevel 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.

[27] The SSLE was implemented on a parallel computing platform using the LINUX operating system; the interpretation of the hydraulic tomography tests was carried out

Figure 11. Variograms of (a) the estimated hydraulic conductivity and true fields and (b) the estimated specific storage and true fields in the 3-D aquifer.

Table 1. Comparison of Statistical Properties of the 3-D Aquifer

	True lnK	Estimated lnK	True $\ln S_s$	Estimated lnS.
Mean	-1.079	-0.96	-8.52	-8.47
Variance	0.50	0.30	0.10	0.06
Horizontal correlation scale, m	20	30	20	35
Vertical correlation scale, m				

using a 10-node PC cluster (Pentium 4, 2.8 GHz CPU each); the total computing time for the interpretation was 610 minutes.

[28] Figures 8a, 8b, 8c, and 8d plot the estimated hydraulic conductivity after two, four, six, and eight pumping tests, respectively, and the true hydraulic conductivity field is shown in Figure 8e. The estimated specific storage fields after two, four, six, and eight pumping tests are illustrated in Figures 9a, 9b, 9c, and 9d, with the true field shown in Figure 9e. Both Figures 8 and 9 show that the general pattern of heterogeneity of the aquifer was already captured by just from the first two pumping tests; after eight pumping tests greater details were revealed, but the improvement rate diminished as more pumping tests were conducted.

[29] Figure 10a shows a frequency distribution with the mean and variance of the difference between the true log hydraulic conductivity field and that estimated (i.e., estimation errors) after eight pumping tests and the distribution of the estimation error of log specific storage and their mean and variance are illustrated in Figure 10b. The error distributions are approximately normal, indicative of unbiasness of our estimator. The slight bias in the estimates can be attributed to the effective nature of the estimated parameters [Yeh et al., 1996; Hanna and Yeh, 1998]. The horizontal and vertical variograms of estimated and true hydraulic conductivity and specific storage fields are depicted in Figures 11a and 11b, respectively. Generally speaking, variograms of the estimates have similar spatial patterns as those of the true fields, in both horizontal and vertical directions. The variances of the estimates are expected to be lower and their correlation scales were longer than true ones (see Table 1). This difference is due to the conditional expectation approach embedded in the SSLE method and insufficient data.

[30] 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 instability 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 by Yeh and Liu [2000].

4. Conclusions

[31] The 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. 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.

[32] The cross correlation analysis shows that the correlation between head and specific storage is high at early time, diminishes rapidly with time, and is confined to the vicinity of the head observation location. On the contrary, the correlation between head and hydraulic conductivity increases and the area with high correlations broadens with time. To simultaneously estimate hydraulic conductivity and specific storage parameters, head data at both early and late times thus should be used.

[33] 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.

[34] 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. More computationally efficient methodologies must be developed to improve the analysis of transient hydraulic tomographic surveys. Finally, a 2-D version of SSLE for the transient hydraulic tomography is available at http://tian.hwr.arizona. edu/yeh/download.

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