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Technical Note

# A method based on local approximate solutions (LAS) for inverting transient flow in heterogeneous aquifers

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SUMMARY

An inverse method based on local approximate solutions (LAS inverse method) is proposed to invert transient flows in heterogeneous aquifers. Unlike the objective-function-based inversion techniques, the method does not require forward simulations to assess measurement-to-model misfits; thus the knowledge of aquifer initial conditions (IC) and boundary conditions (BC) is not required. Instead, the method employs a set of local approximate solutions of flow to impose continuity of hydraulic head and Darcy fluxes throughout space and time. Given sufficient (but limited) measurements, it yields well-posed systems of nonlinear equations that can be solved efficiently with optimization. Solution of the inversion includes parameters (hydraulic conductivities, specific storage coefficients) and flow field including the unknown IC and BC. Given error-free measurements, the estimated conductivities and specific storages are accurate within 10% of the true values. When increasing measurement errors are imposed, the estimated parameters become less accurate, but the inverse solution is still stable, i.e., parameter, IC, and BC estimation remains bounded. For a problem where parameter variation is unknown, highly parameterized inversion can reveal the underlying parameter structure, whereas equivalent conductivity and average storage coefficient can also be estimated. Because of the physically-based constraints placed in inversion, the number of measurements does not need to exceed the number of parameters for the inverse method to succeed.



## 1. Introduction

The physical principles of groundwater motion are well understood, leading to the establishment of a forward mathematical model solving the groundwater flow equation for a given set of parameters, and under a given set of initial and boundary conditions. When predictions of aquifer responses are needed, however, question arises as to how to estimate the model parameters and assign the appropriate initial and boundary conditions. Such questions are commonly addressed with the inverse method, which according to Sagar et al. (1975), can be characterized into five types based on the types of unknowns to be estimated: (I) model parameters, (II) initial conditions, (III) boundary conditions, (IV) sources and sinks, and (V) a mixture of the above. Because of the well-known importance of parameters in influencing subsurface flow and transport, the majority of the existing inverse methods falls into Type I inversion, and are referred to as "parameter estimation" techniques. In this work, Type V Inversion for transient groundwater flows is of interest, where we aim to simultaneously estimate: (1) model parameters, (2) model initial conditions, and (3) model boundary conditions. Problems with source/sink effects are not addressed here and are left for another treatment.

In modeling transient aquifer responses to natural or imposed forcings, hydraulic conductivity and storage coefficient are key parameters. In Type I inversion, parameter estimation is generally facilitated by the indirect inverse methods which minimize a (regularized) measurement-to-model misfit or an objective function (e.g., Hughson and Yeh, 2000; Cardiff et al., 2012; Li et al., 2005; Zhu and Yeh, 2005; Liu et al., 2007; Berg and Illman, 2011; Mao et al., 2013; Zhou et al., 2014). By building and calibrating a forward model, model fit against observations is iteratively improved until both conductivity and storage coefficient can be determined. Because a forward model is needed for evaluating the objective function, aquifer initial conditions (IC) and boundary conditions (BC) both need to be ascertained prior to parameter estimation (and the forward simulations). However, due to data limitation in accessing the subsurface, aquifer initial and boundary conditions are often poorly known.

This study presents a direct inverse method for inverting transient flows in heterogeneous aquifers with spatially varying parameters. Based on time-varying observations such as hydraulic

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heads and Darcy fluxes, aquifer hydraulic conductivit(ies), specific storage(s), BC, and IC are simultaneously estimated. The direct method extends steady state inversion methods developed in previous works (Irsa and Zhang, 2012; Zhang, 2013; Jiao and Zhang, 2014; Zhang et al., 2014), where analytical solutions of the steady state flow equation were used to enforce local fluid flow continuity in space (i.e., the continuity constraint). For transient flow, however, analytical solutions flexible enough to account for general heterogeneous problems where aquifer flows can be significantly influenced by (nearby) boundary characteristics do not exist. Thus, local approximate solutions (LAS) are proposed in this study to enforce fluid flow continuity in both space and time. To honor flow physics, an equation constraint is imposed at selected points in space and time to ensure that the transient flow equation is approximately satisfied. For both steady-state and transient inversion, the local exact or approximate solutions are conditioned by (limited) measurements (i.e., the data constraint). These constraints give rise to a system of linear or nonlinear equations which can be assembled and solved in a single step with optimization techniques. The direct inverse method is therefore computationally efficient, as repeated forward simulations are not required, nor is the knowledge of aquifer initial and boundary conditions. The local flow solutions and aquifer parameters are simultaneously estimated, from which hydraulic head and flow fields (including the unknown IC and BC) can be determined. Herein, to distinguish the transient technique from the earlier steady state methods, it is referred to as the "LAS inverse method".

Using one-dimensional (1D) synthetic aquifer problems with heterogeneous distributions of hydraulic conductivity and specific storage, accuracy and stability of the LAS inverse method is demonstrated. The inverse solution is considered stable if increasing measurement errors do not lead to unbounded parameter, IC, and BC estimation errors. For a problem where parameter variation is unknown, highly parameterized inversion can be carried out, whereas conductivity is estimated for each inversion grid cell. For a heterogeneous problem where inverse parameterization assumes homogeneity, equivalent conductivity and average storage coefficient can be determined.

## 2. Theory

For transient flow in a 1D confined aquifer, the governing continuity and momentum equations can be written as:

$$S_s(z)\frac{\partial h(z,t)}{\partial t} = \frac{\partial}{\partial z}\left(K(z)\frac{\partial h(z,t)}{\partial z}\right) \quad on \quad \Omega \tag{1}$$

$$q(z,t) = -K(z)\frac{\partial h(z,t)}{\partial z} \quad on \quad \Omega \tag{2}$$

where $S_s(z)$ is specific storage $[1/L]$, $h(z,t)$ is hydraulic head $[L]$, $K(z)$ is hydraulic conductivity $[L/T]$, $\Omega$ is the solution domain, $z$ is vertical axis $[L]$, $t$ is time $[T]$, $q(z,t)$ is vertical Darcy flux $[L/T]$. $S_s$ and $K$ are both spatially variable. The above equations are written for the vertical axis, although the technique of this study can be extended to any coordinate direction as well as to higher dimensions.

Given $S_s(z)$, $K(z)$, and a set of initial and boundary conditions, Eqs. (1) and (2) can be solved in the forward mode. The initial conditions of the forward model are $h(z,t_0)$. In the forward models solved in this study, Dirichlet BC are assigned to the boundaries: $h = g(z,t)$ *on* $\Gamma$, where $\Gamma$ is Dirichlet-type model boundary, and $g(z,t)$ describes a set of prescribed heads on $\Gamma$.

Eqs. (1) and (2) can be expressed in dimensionless form as:

$$S_s^*\frac{\partial H^*(Z^*,T^*)}{\partial T^*} = \frac{\partial}{\partial Z^*}\left(K^*\frac{\partial H^*(Z^*,T^*)}{\partial Z^*}\right) \tag{3}$$

$$Q^* = -K^*\frac{\partial H^*(Z^*,T^*)}{\partial Z^*} \quad Z^* \in [0,1], \quad T^* \in [0,+\infty] \tag{4}$$

where $H^* = \frac{h(z,t)}{H}$, $Z^* = \frac{z}{Z}$, $T^* = \frac{t}{T}$, $S^* = S_sH$, and $K^* = \frac{KHT}{Z^2}$. $H$ is a reference hydraulic head, $Z$ is total thickness of the aquifer, $t$ is total simulation time, and $T$ is output time interval in forward simulation (to generate observations for inversion). $S_s^*$, $K^*$, $H^*$, $Z^*$, $Q^*$ and $T^*$ are dimensionless specific storage, hydraulic conductivity, hydraulic head, $z$ axis, Darcy flux, and time, respectively. These variables will be used in inversion with results ($K^*$, $S_s{}^*$, $H^*$) expressed in dimensionless forms. Again, $S_s{}^*$ and $K^*$ are both spatially variable.

### 2.1. The LAS inverse method

The inverse method enforces three sets of constraints: (1) global continuity of hydraulic head and Darcy fluxes throughout the solution domain at each discretized time in inversion; (2) local conditioning of LAS to observed hydraulic heads and Darcy fluxes at the same discretized time; (3) an equation constraint at selected points in space and time (below). The continuity equations, as the first constraint, are written as:

$$\int \left[H_i^{*n}(\Gamma_j) - H_k^{*n}(\Gamma_j)\right]\delta^n(p_j-\varepsilon)d\Gamma_j = 0, \quad j = 1,\ldots,Y; \quad n = 1,\ldots,X \tag{5}$$

$$\int \left[Q_i^{*n}(\Gamma_j) - Q_k^{*n}(\Gamma_j)\right]\delta^n(p_j-\varepsilon)d\Gamma_j = 0, \quad j = 1,\ldots,Y; \quad n = 1,\ldots,X \tag{6}$$

where $n$ denotes a discretized time in inversion, $Y$ is total number of cell interfaces in the inversion grid, $X$ is total number of time steps, and $H^{*n}$ and $Q^{*n}$ are the fundamental solutions of inversion at the $n$th time, and $i$ and $k$ denote cells in the inversion grid adjacent to the $j$th interface ($\Gamma_j$) at the $n$th time. $\delta^n(p_j-\varepsilon)$ is a Dirac delta weighting function at the $n$th time which samples the residuals at a set of collocation points $p_j$ on $\Gamma_j$.

At each discretized time, the fundamental solutions are conditioned by measurements:

$$\delta^n(p_a-\varepsilon)\left(H^{*n}(p_a) - H_o^{*n}\right) = 0, \quad a = 1,\ldots,A; \quad n = 1,\ldots,X \tag{7}$$

$$\delta^n(p_b-\varepsilon)(Q^{*n}(p_b) - Q_o^{*n}) = 0, \quad b = 1,\ldots,B; \quad n = 1,\ldots,X \tag{8}$$

where $p_a$ and $p_b$ are a set of measurement points, $H_o^{*n}$ and $Q_o^{*n}$ are observed dimensionless hydraulic head and Darcy flux at the $n$th time at $p_a$ and $p_b$, respectively, $A$ and $B$ are the number of observed heads and fluxes at the $n$th time, respectively, $\delta^n(p_a-\varepsilon)$ and $\delta^n(p_b - \varepsilon)$ are weighting functions assigned to the equations to reflect the magnitude of the measurement errors at the $n$th time.

For transient flow, the equation constraints are used to enforce the flow physics locally in space and time:

$$\delta^n(p_c-\varepsilon)\left[S_s^*\frac{\partial H^*(Z^*,T^*)}{\partial T^*} - \frac{\partial}{\partial Z^*}\left(K^*\frac{\partial H^*(Z^*,T^*)}{\partial Z^*}\right)\right]\Bigg|_{n,c} = 0 \tag{9}$$

$$c = 1,\ldots,Y+A+B; \quad n = 1,\ldots,X$$

where $p_c$ include both the collocation points and the measurement location. The equation residual $R = S_s^*\frac{\partial H^*(Z^*,T^*)}{\partial T^*} - \frac{\partial}{\partial Z^*}\left(K^*\frac{\partial H^*(Z^*,T^*)}{\partial Z^*}\right)$ is minimized at $p_c$ at each discretized time. Transient inversion requires Eq. (9) because the fundamental solutions ($H^*$ and $Q^*$) are approximate rather than exact. Exact solutions for transient flows exist (e.g., Theis solution), but they are developed under restrictive assumptions, e.g., homogeneous parameters and infinite aquifer boundaries. Using approximate solutions allows the evaluation of more general problems, where parameters are heterogeneous and BC or IC influence on flow can be significant.

*2.2. Fundamental solutions*

The inverse method adopts a set of fundamental solutions of inversion which are applicable to describing flow in a homogeneous sub-domain ($\Omega_i$) of the full solution domain, e.g., individual inversion grid cells or individual hydrofacies. Within each $\Omega_i$, parameters (i.e., $S_s^*$ and $K^*$) are homogeneous and Eqs. (3) and (4) become:

$$S_s^* \frac{\partial H^*(Z^*, T^*)}{\partial T^*} = K^* \frac{\partial}{\partial Z^*}\left(\frac{\partial H^*(Z^*, T^*)}{\partial Z^*}\right) \quad on \quad \Omega_i \tag{10}$$

$$Q^* = -K^* \frac{\partial H^*(Z^*, T^*)}{\partial Z^*} \quad on \quad \Omega_i \tag{11}$$

where $K^*$, $S_s^*$, $H^*$, and $Q^*$ are dimensionless variables of the sub-domain ($S_s^*$ and $K^*$ are unknown parameters). For the solution of Eqs. (10) and (11), polynomial functions of hydraulic head and Darcy flux are proposed as the LAS which depend on the dimensionless space ($Z^*$) and time ($T^*$):

$$\begin{aligned} H^*(Z^*, T^*) = {} & a_1 + a_2 T^* + a_3 T^{*2} + (a_4 + a_5 T^* + a_6 T^{*2}) Z^* + (a_7 \\ & + a_8 T^* + a_9 T^{*2}) Z^{*2} + (a_{10} + a_{11} T^* + a_{12} T^{*2}) Z^{*3} \end{aligned} \tag{12}$$

$$\begin{aligned} Q^*(Z^*, T^*) = {} & -K^*((a_4 + a_5 T^* + a_6 T^{*2}) + (a_7 + a_8 T^* + a_9 T^{*2}) Z^* \\ & + (a_{10} + a_{11} T^* + a_{12} T^{*2}) Z^{*2}) \end{aligned} \tag{13}$$

where $a_i (i = 1, \ldots, 12)$ are the unknown coefficients to be determined by inversion. After discretizing Eq. (10) over the solution domain, the coefficients become cell-wise constants: $[\boldsymbol{x}^T = a_i^l, K^{*m}, S_s^{*p}]$, where $\boldsymbol{x}$ is the inverse solution, $i = 1, \ldots, 12$, $l = 1, \ldots, M$ (number of inversion grid cells), $m = 1, \ldots, R$ (number of hydraulic conductivity zones), $p = 1, \ldots, P$ (number of specific storage zones). For 1D transient flows, polynomial functions are adopted, although other functions can potentially be explored to address more complex problems. Given Eqs. (12) and (13), the residual of Eq. (9) can be rewritten as:

$$\begin{aligned} R_c^n = {} & S_s^*[a_2 + 2a_3 T^* + (a_5 + 2a_6 T^*) Z^* + (a_8 + 2a_9 T^*) Z^{*2} \\ & + (a_{11} + 2a_{12} T^*) Z^{*3}] - K^*[2(a_7 + a_8 T^* + a_9 T^{*2}) \\ & - 6(a_{10} + a_{11} T^* + a_{12} T^{*2}) Z^*] \end{aligned} \tag{14}$$

Given Eqs. (12)–(14), for each discretized time in inversion, Eqs. (5) and (6) are written at the collocation points, Eqs. (7) and (8) are written at the measurement location, and Eq. (9) imposes the physical flow constraints at both the collocation points and the measurement location. For all discretized times, a single inversion system of equations is assembled, which can be solved with optimization (Jiao and Zhang, 2014). The above procedure is referred to as LAS inversion.

## 3. Results

Using one-dimensional forward models with heterogeneous hydraulic conductivity and specific storage, accuracy and stability of inversion is tested. The inverse solution is considered stable if increasing measurement errors do not lead to unbounded parameter, IC, and BC estimation errors. Inverse parameterization is first assumed identical to the true parameter fields, then flow fields with unknown parameter structures are inverted. In the later cases, inversion aims to (1) identify parameter structure using highly parameterized estimation; (2) identify equivalent or average parameters. The inverse solution is verified by comparing the estimated parameters ($S_s^*$ and $K^*$) and the recovered hydraulic heads to the forward (true) models. The forward models are simulated with the finite-difference method (FDM) to generate observations under a set of true model IC and BC. Two FDMs are created assuming typical sandstone properties, while sharing the same initial conditions (i.e., a parabolic function with a range of 1–2, with $H^* = 1$ at the boundaries and $H^* = 2$ at $Z^* = 0.5$), boundary conditions ($H^*(0,T^*) = H^*(1,T^*) = 1$), computational domain ($Z^* \in [0, 1]$), spatial discretization (200 grid cells), and temporal discretization ($\Delta t = T/50$). To each model, different hydraulic conductivity and specific storage are assigned. Observations are generated at 3 dimensionless output times (i.e., $T^* = 1$–3), based on which a set of inverse analyses is carried out using a uniform grid with 10 cells (i.e., with a dimensionless discretization of 0.1).

In the first analysis, the FDM contains 4 conductivity zones and 2 specific storage zones. The conductivity zones ($K1^*$–$K4^*$) are divided at $Z^* = 0.3$, 0.5, 0.7; the storage zones are divided at $Z^* = 0.5$. The true parameters are listed in Table 1. The true hydraulic head profiles at $t_0$ and each output time are shown in Fig. 1 (solid curves). The observations include (1) 60 heads sampled from the FDM at the dimensionless output times of $T^* = 1$–3. At each $T^*$, 20 heads were evenly sampled, i.e., each inversion grid cell had 2 observed heads. Over time, the same head measurement location is used. (2) 12 Fluxes sampled at the same output times (for each $T^*$, 4 fluxes were sampled). Over time, the same flux measurement location is used. None of the observations lies on the model boundaries, nor are they sampled at the initial time. Stability analysis is first conducted to evaluate the accuracy of inversion under increasing head measurement errors. To impose such errors, $H^{*m} = H^{*FDM} \pm \Delta H^*$, where $H^{*m}$ is measured head provided to inversion, $H^{*FDM}$ is error-free head (rendered dimensionless) from the FDM, and $\Delta H^*$ is a dimensionless error. The highest error imposed is ±2% of the total head variation in the FDM. For example, for a problem with a vertical dimension of 100 m, a hydraulic gradient of 1% yields a total head change of 1 m. The measured heads will therefore vary within ±2 cm of the true values. Modern tapes and pressure transducers can yield observed heads with a precision of <1 cm (Post and von Asmuth, 2013), head measurement errors up to ±2% are thus considered reasonable. Darcy fluxes sampled from the FDM are not subject to errors.

When error-free heads and heads with ±0.5% errors are provided to inversion, the estimated conductivities and specific storages are close to those of the FDM, i.e., the absolute relative errors of parameter estimation ($|K^{*FDM} - K^{*est}|/K^{*FDM}$ and $|S_s^{*FDM} - S_s^{*est}|/S_s^{*FDM}$) are less than 20% (Table 1). When error-free data are used, the inverted head profiles are very accurate compared to the true heads (Fig. 1). When head measurement errors are increased, the estimated specific storages and conductivities become less accurate (Table 1), but the inverted heads are stable (Fig. 1). The inverse solution adequately recovers the IC at $T^* = 0$, even though no measurements were sampled at this time. For all levels of the measurement errors, deviation of the inverted heads from the FDM heads is greatest at $T^* = 0$ (the IC), but becomes smaller at later times. The higher estimation errors may be due to spatial and temporal *extrapolation* of the LAS to $T^* = 0$. Moreover, at all dimensionless output times, the hydraulic head BC at $Z^* = 0$ and $Z^* = 1$ are recovered well despite the fact that no measurements were sampled at the boundaries.

Next, a homogeneous FDM is simulated ($K^* = 1.0 \times 10^{-4}$; $S_s^* = 5.0 \times 10^{-3}$) from which 60 heads and 30 fluxes were sampled at the same 3 dimensionless output times. At each time, 20 error-free heads and 10 fluxes were sampled and none lied on the boundaries. When error-free heads are provided to inversion, ten conductivities and one specific storage are estimated with good

**Table 1**
Parameter estimation for a confined aquifer under increasing measurement errors. The true parameters of the forward FDM is also shown.

| | $K^*$ | | | | $S_s^*$ | | Number of Grid Cells |
|---|---|---|---|---|---|---|---|
| | $K1^*$ | $K2^*$ | $K3^*$ | $K4^*$ | $S_{s1}^*$ | $S_{s2}^*$ | |
| FDM | $1.0 \times 10^{-3}$ | $5.0 \times 10^{-4}$ | $1.0 \times 10^{-4}$ | $2.0 \times 10^{-4}$ | $1.0 \times 10^{-2}$ | $5.0 \times 10^{-3}$ | 200 |
| (0% error) | $9.9 \times 10^{-4}$ | $4.9 \times 10^{-4}$ | $1.1 \times 10^{-4}$ | $2.0 \times 10^{-4}$ | $1.1 \times 10^{-2}$ | $5.7 \times 10^{-3}$ | 10 |
| (±0.5% error) | $1.0 \times 10^{-3}$ | $4.9 \times 10^{-4}$ | $1.1 \times 10^{-4}$ | $2.1 \times 10^{-4}$ | $1.2 \times 10^{-2}$ | $6.0 \times 10^{-3}$ | 10 |
| (±1% error) | $1.1 \times 10^{-3}$ | $4.8 \times 10^{-4}$ | $1.2 \times 10^{-4}$ | $2.1 \times 10^{-4}$ | $1.2 \times 10^{-2}$ | $6.5 \times 10^{-3}$ | 10 |
| (±2% error) | $1.2 \times 10^{-3}$ | $4.6 \times 10^{-4}$ | $1.2 \times 10^{-4}$ | $2.3 \times 10^{-4}$ | $1.9 \times 10^{-3}$ | $6.5 \times 10^{-3}$ | 10 |

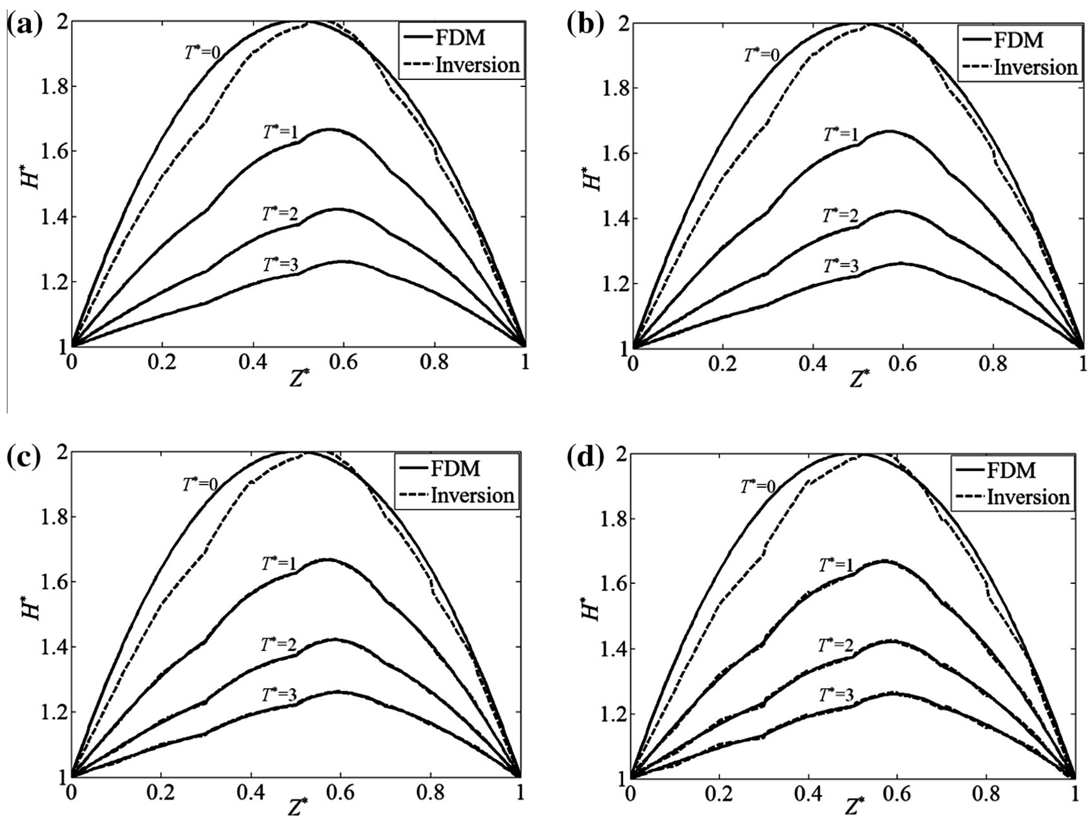


**Fig. 1.** Inverted hydraulic heads versus FDM hydraulic heads at $T^*$ = 0–3. Increasing errors are imposed on the observed heads: (a) error-free; (b) ±0.2%; (c) ±1% and (d) ±2%.

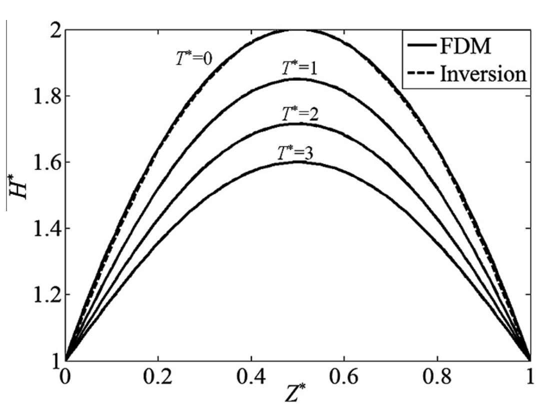


**Fig. 2.** Highly parameterized inversion results for a homogeneous problem: inverted hydraulic heads (using error-free measurements) versus FDM hydraulic heads at $T^*$ = 0–3.

accuracy, i.e., $K^*$ range from $9.3 \times 10^{-5}$ to $1.1 \times 10^{-4}$ and the single $S_s{}^*$ is estimated as $4.4 \times 10^{-3}$. In this case, $K^*$ are more accurately estimated (absolute relative errors are less than 7%) and the underlying conductivity field is revealed by inversion to be homogeneous. In Fig. 2, the inverted heads are also favorably compared to the FDM heads. Again, both the FDM initial and boundary conditions are accurately recovered.

Given the FDM and observations of the first analysis (i.e., heterogeneous true model), the inverse analysis is repeated assuming homogeneous parameters. Only a single conductivity and a single specific storage were estimated. Given error-free measurements, inversion yields: $K^* = 7.3 \times 10^{-4}$ and $S_s{}^* = 5.1 \times 10^{-4}$, which are not far from the analytical equivalent conductivity ($2.4 \times 10^{-4}$) and average specific storage ($7.5 \times 10^{-3}$) independently computed from the forward model. Exact equivalent parameters cannot be obtained because inversion is conditioned to limited observations in space and time.

## 4. Conclusion

An inverse method based on local approximate solutions (LAS) is proposed to invert transient flows for a confined aquifer without the knowledge of its initial and boundary conditions. LAS are imposed to ensure continuity of hydraulic head and Darcy fluxes throughout space and time. By conditioning these solutions to observed heads and fluxes, parameters (hydraulic conductivity and specific storage), boundary conditions, and initial conditions can be simultaneously estimated under a set of equation constraints that enforce flow physics at selected points in space and time. For forward problems with parameters ranging from homogeneous to heterogeneous, accuracy and stability of the LAS inverse method is demonstrated. Key results are summarized as follows: (1) transient inversion is stable under increasing head measurement errors; (2) when error-free observations are used to condition the inversion, the estimated hydraulic conductivities and specific storages are accurate within 10% of the true values; (3) aquifer initial and boundary conditions can be accurately recovered even though no measurements were sampled at $t_0$ and at the boundaries; (4) for problems with unknown parameter variation, highly parameterized conductivities can be estimated which reveal the underlying parameter structure, while physically reasonable, equivalent conductivity and average specific storage can also be estimated; (5) the number of (spatial and temporal) head and flux observations can be fewer than the number of unknown parameters, because LAS inversion is constrained by (a) measurements, (b) continuity equations, and (c) equation constraints to enforce flow physics. The LAS inverse method thus shows promise for characterizing data-poor subsurface systems.

In this work, measurements provided to inversion include hydraulic heads and Darcy fluxes monitored over time. While head measurements can be easily obtained with multilevel pressure transducers, in situ groundwater flux sampling requires specialized techniques (Labaky et al., 2009). Only hydraulic data are used to condition the inversion. Future work will address joint inversion with indirect measurements. Future work will also extend the technique of this study to higher spatial dimensions.

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