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Three-dimensional aquifer inversion under unknown boundary conditions

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SUMMARY

A new method for three-dimensional steady-state aquifer inversion is developed to simultaneously estimate aquifer hydraulic conductivities and the unknown aquifer boundary conditions (BC). The method has its key strength in computational efficiency, as there is no need to fit an objective function, nor repeated simulations of a forward flow model. It employs a discretization scheme based on functional approximations and a collocation technique to enforce the global flow solution. The noisy observed data are directly incorporated into the inversion matrix, which is solved in a one-step procedure. The inverse solution includes hydraulic conductivities and head and flux approximating functions from which the model BC can be inferred. Thus a key advantage of the method is that it eliminates the non-uniqueness associated with parameter estimation under unknown BC which can cause the result of inversion sensitive to the assumption of aquifer BC. Two approximating functions are tested here, one employing quadratic approximation of the hydraulic head (flux is linear), the other cubic approximation. Two different BC are also tested, one leading to linear flow, the other strongly nonlinear flow. For both BC, the estimated conductivities converge to the true values with grid refinement, and the solution is accurate and stable when a sufficient number of the observation data is used. Compared to the quadratic function, the cubic function leads to a faster convergence of the estimated conductivity at a lower level of grid discretization, while it is also more robust for the different flow conditions tested. A sensitivity analysis is conducted whereby the inversion accuracy is evaluated against data density. Composite scale sensitivity (CSS) can reveal the overall information content of the data. However, when the number of measurements is fixed, CSS cannot reveal whether the observed data can lead to reliable conductivity estimates. A one-observation-at-a-time (OAT) approach is proposed, which can indicate the reliability of the estimated conductivity for a given set of the observation data. To evaluate the stability of the method when the observation data contain errors, a problem with 4 hydrofacies conductivities is inverted using hydraulic heads and a single Darcy flux component. The results are accurate when the measurement error is small but become slightly less accurate when the error is larger. In summary, flow condition, inverse formulation, grid discretization, observation data density and location, and measurement errors all influence the accuracy of inversion.

1. Introduction

Hydraulic conductivity (K) is a critical parameter influencing fluid flow and solute transport in aquifers. However, estimation of aquifer hydraulic conductivity is a challenging task, due to issues related to aquifer heterogeneity, parameter and measurement scale effect, uncertainty in aquifer boundary conditions, and the lack of efficient estimation techniques. This study presents a three-dimensional (3D) steady-state inverse method which efficiently and simultaneously estimates aquifer hydraulic conductivities, flow field, and the unknown aquifer boundary conditions (BC). In the following paragraphs, different approaches of estimating aquifer hydraulic conductivity are briefly reviewed, before key features of the new method are presented and contrasted with the existing inverse methodology.

Aquifer K can be measured directly with Darcy tests on oriented cores or estimated using aquifer tests, indirect means, or via the calibration of an aquifer simulation model. Typically, core conductivity measurements sample a small aquifer volume, leading to values that are not representative of the aquifer at larger scales. With slug tests, K can be estimated for a greater volume using analytical flow solutions developed assuming radial flow from the test well in a homogeneous formation with an infinite lateral extent. Similarly, with pumping tests, analytical flow solutions have been developed

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to estimate large-scale horizontal hydraulic properties, e.g., the well-known Thiem solution for analyzing steady-state flow and the Theis solution for analyzing transient flow (Fitts, 2013). To obtain *K* at higher resolutions, the analytical functions can be applied to specific aquifer intervals that are isolated from the other intervals, e.g., borehole flowmeter test, multilevel slug test, direct-push permeameter test (Molz et al., 1994; Butler, 2005; Bohling et al., 2012). Compared to the *K* derived from core measurement and pumping test, these measurements can sample an intermediate range of the formation volume. Moreover, at the same core scale or well-test intervals, indirect *K* measurements can be made based on correlations between rock petrophysical properties and fluid flow properties, e.g., magnetic resonance logs, acoustic, density, or neutron logs, and electrical-conductivity profiling (Williams et al., 1984; Tang and Cheng, 1996; Shapiro et al., 1999; Hyndman et al., 1994, 2000; Schulmeister et al., 2003; Kobr et al., 2005; Camporese et al., 2011). For quality control, these indirect measurements are compared and combined with one or more direct *K* measurements. However, correlation between fluid flow and petrophysical properties is often site-specific and empirical in nature. To address this issue, joint inversion techniques have been developed whereas aquifer hydrodynamic data are analyzed jointly with geophysical measurements (Kowalsky et al., 2006; Brauchler et al., 2012). In these analyses, explicit correlation functions are not needed, although certain "structure similarity" between fluid flow and petrophysical properties is enforced to help constrain the joint inversion.

Another type of indirect *K* measurement can be made by building and calibrating an aquifer simulation model with an inverse method (Hill and Tiedeman, 2007). For an overview of the inverse methodologies used in groundwater model calibration, including both direct and indirect methods and their pros and cons, please see Neuman and Yakowitz (1979), Weir (1989), and Irsa and Zhang (2012). Within the inversion framework, *K* becomes a model calibration parameter and can be estimated (or inverted) at different scales of interest. For example, aquifer flow models with distinct hydrofacies zones can be built for which *K* can be estimated for each hydrofacies. In highly parameterized inversion, *K* can be estimated for each grid cell by imposing additional constraint equations on the inverse formulations (Zimmerman et al., 1998; Doherty, 2005; Liu and Kitanidis, 2011). However, most of the existing inverse techniques are based on minimizing an objective function, which is typically defined as a form of mismatch between the measurement data and the corresponding model simulated values. During inversion, to minimize the objective function, parameters including conductivities are updated iteratively using a forward model which provides the linkage between the parameters and the data. Because a forward model is needed, boundary conditions (BC) of the model are commonly assumed known, or less frequently, calibrated during the inversion. However, BC of natural aquifers are often unknown or uncertain. (In transient problems, both aquifer initial and boundary conditions are unknown.) As demonstrated by Irsa and Zhang (2012), different combinations of parameters and BC can lead to the same objective function values, thus results of many existing techniques may become non-unique.

To address non-uniqueness in *K* estimation, Irsa and Zhang (2012) developed a novel steady-state direct method for inverting two-dimensional (2D) confined aquifer flow. The method adopts a set of approximating functions of hydraulic heads and groundwater fluxes as the fundamental solutions of inversion. It does not rely on minimizing objective functions (i.e., forward model-data mismatch), while hydraulic conductivity, flow field, and the unknown aquifer BC can be simultaneously estimated. Synthetic aquifer problems with regular and irregular geometries, different (deterministic) hydrofacies patterns, variances of heterogeneity, and error magnitudes were tested. In all cases, *K* converged to the true or expected values and was therefore unique, based on which heads and flow fields were reconstructed directly via the approximating functions. Boundary conditions were then inferred from these fields. In the 2D analysis, the inversion accuracy was demonstrated to improve with increasing observed data, low measurement errors, and grid refinement, although source/sink effects cannot be accommodated. To address the source/sink effects (e.g., pumping and recharge), Zhang (submitted for publication) extended the technique to inverting unconfined aquifers by superposing analytical flow solutions to generate the approximating functions. In these cases, the inverse solution was obtained via nonlinear optimization while the same high computation efficiency was maintained. Furthermore, to account for uncertainty in inversion due to the uncertain hydrofacies patterns, the method was combined with geostatistical simulation, whereas both *K* uncertainty and uncertainty in the unknown aquifer BC can be quantified (Wang et al., 2013).

This study extends our earlier works by demonstrating the applicability of the new direct method to inverting three-dimensional (3D) steady-state flow in confined aquifers. Similar to our earlier works, the 3D algorithm is tested using a set of synthetic forward (true) models which provide the measurement data, with or without measurement errors, for inversion. However, unlike the earlier works, the inversion accuracy is tested using two different sets of (increasingly complex) approximating functions under two different global flow BC which induce either linear or strongly nonlinear flow. Again, BC of the forward models are assumed unknown and are estimated by inversion along with the hydraulic conductivities and the flow field. To assess the accuracy of inversion, the estimated conductivities and the BC are compared to those of the forward models. A sensitivity analysis is conducted to evaluate how the inversion outcomes converge to the true model with grid refinement or with increasing observation data. The issue of data worth is examined using different statistical measures. The stability of the method is also examined when measurement errors are increased from error-free to a set of realistic values. The inverse solution is considered stable if the estimated hydraulic conductivities do not vary from the true values by more than one orders of magnitude.

In the reminder of this article, non-uniqueness in parameter estimation under unknown aquifer BC is first illustrated, before the 3D inverse formulation of this study is introduced. Results are presented in four sections relating to: (1) convergence of the inverse algorithm with grid refinement; (2) data needs; (3) information content of the observations; and (4) stability of inversion under increasing measurement errors. In addressing topics (1)–(3), a homogeneous aquifer problem is inverted and the observation data include hydraulic heads and a single groundwater flow rate. In addressing topic (4), inversion is carried out for a heterogeneous problem with 4 hydrofacies. In this case, observation data include hydraulic heads and a single Darcy flux component. The relevant results are discussed before conclusion and future research are summarized at the end.

2. Non-uniqueness in parameter estimation

The determination of hydraulic conductivity for steady-state groundwater flow is mainly driven by the indirect inverse methods solving a set of boundary value problems to minimize an objective function. These methods assume either known BC for a given problem, or by appropriate parameterizations, obtain optimized BC during inversion which is typically an iterative procedure. The earlier generation of direct inversion methods (e.g., see a review in Sun (1994)) make similar assumptions about the BC, although