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Three-dimensional geostatistical inversion of synthetic tomographic pumping and heat-tracer tests in a nested-cell setup

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ABSTRACT

A main purpose of groundwater inverse modeling lies in estimating the hydraulic conductivity field of an aquifer. Traditionally, hydraulic head measurements, possibly obtained in tomographic setups, are used as data. Because the groundwater flow equation is diffusive, many pumping and observation wells would be necessary to obtain a high resolution of hydraulic conductivity, which is typically not possible. We suggest performing heat tracer tests using the same already installed pumping wells and thermometers in observation planes to amend the hydraulic head data set by the arrival times of the heat signals. For each tomographic combinations of wells, we recommend installing an outer pair of pumping wells, generating artificial ambient flow, and an inner well pair in which the tests are performed. We jointly invert heads and thermal arrival times in 3-D by the quasi-linear geostatistical approach using an efficiently parallelized code running on a mid-range cluster. In the present study, we evaluate the value of heat tracer versus head data in a synthetic test case, where the estimated fields can be compared to the synthetic truth. Because the sensitivity patterns of the thermal arrival times differ from those of head measurements, the resolved variance in the estimated field is 6 to 10 times higher in the joint inversion in comparison to inverting head data only. Also, in contrast to head measurements, reversing the flow field and repeating the heat-tracer test improves the estimate in terms of reducing the estimation variance of the estimate. Based on the synthetic test case, we recommend performing the tests in four principal directions, requiring in total eight pumping wells and four intersecting observation planes for heads and temperature in each direction.

1. Introduction

Estimating the spatial distribution of hydraulic conductivity in a heterogeneous aquifer is a remaining challenge of subsurface hydrology. The spatial variability of hydraulic conductivity highly influences flow and solute transport in the subsurface. Simulations based on an effective mean value of hydraulic conductivity lead to biased estimates of plume spreading [27,45,54], which may cause failure in subsurface remediation.

Since direct measurements of hydraulic conductivity are scarce and local, and require sampling, hydraulic conductivity is typically inferred from measurements of quantities depending on conductivity, such as hydraulic heads, potentially monitored during hydraulic tests, and tracer test data. Conventional approaches of parameter estimation, such as the type-curve approach for pumping tests [31], fail in estimating the spatial distribution of hydraulic conductivity, since they are based on the assumption of homogeneity, even if analyzing pumping-test data from different wells in the same aquifer yields different effective parameters [34,35,57]. In contrast, inverse methods are capable of estimating hydraulic conductivity as spatially variable fields, taking into account the spatial sensitivities of the data with respect to the estimated parameters. In particular, geostatistical inverse approaches, assume that the log-hydraulic conductivity is a random space function with known correlation structure and provide estimates of parameter uncertainty, which may be as important as the estimate itself [3,15,16,22,28,53,56,62,64].

In numerical applications, the spatial domain is discretized into elements or cells. In geostatistical inversion, we assign each cell one parameter set, which may result – depending on the model size – in several million parameters to be estimated in typical three-dimensional applications, while the number of measurements may be within the order of hundreds. This highly underdetermined problem is regularized in geostatistical inversion by considering spatial correlation as prior knowledge. Penalizing non-smoothness of the estimates by Tikhonov regularization results in mathematical expressions equivalent to geostatistical regularization [29,42]. Regardless of the regularization applied, however, any (non-corrupted) additional measurement appears

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valuable for the inverse procedure because the original inverse problem is under-determined.

With the groundwater flow equation being a diffusion equation, high resolution in inverting head data can only be achieved when considering many pumping and observation wells, which may be costly. Unlike hydraulic heads, arrival times of tracers depend on hydraulic conductivity via the convective part of the solute transport equation, resulting in travel time to resemble the integral of inverse hydraulic conductivity along the path leading to the observation point. This implies that the same set of wells can be used for different measurement types with different information content, like in hydraulic tomography setups. In previous studies, we have considered temporal moments of solute-tracer data for this purpose, either measured directly [18,48], or via geoelectrical monitoring [50–52]. These previous studies were restricted to two-dimensional laboratory setups, whereas in the present study, we perform a fully three-dimensional analysis and systematically investigate the information content of (thermal) tracer test data in comparison to head measurements.

Rather than analyzing classical solute tracer tests, we consider the injection of heat as a tracer. This has the advantage that no artificial compound is introduced into the environment. Causing temperature difference of about ±10 Kelvin (K) may be considered environmentally harmless, so that obtaining permissions from regulating agencies may be easier for heat-tracer than for solute-tracer tests. A further advantage is that the temperature can be very easily measured by in situ measurements at a very large number of locations, i.e., without the need of labor intensive sampling or tracer analysis. Also, the high thermal diffusivity has two main advantages. First, it allows a faster repetition of thermal tests because the signal disappears faster than a comparable solute signal. Second, the numerical stability of solving the transport equation for point like sources is increased. The high thermal diffusivity also poses the biggest problem of thermal tracer tests, because the thermal signal disappears over wide distances. In contaminated aquifers, extensive pumping needed for heat-tracer tests may not be possible without expensive water treatment. Another potential disadvantage is that the thermal signal of the tracer test may overlap with the thermal signal from the ground surface [43]. To minimize this disturbance, thermal tracer tests should not be performed in extremely shallow systems where diurnal temperature fluctuations reach the aquifer, and groundwater flow should be accelerated by pumping to reduce the time needed for a single thermal tracer test.

In recent years, hydraulic tomography has been proposed as a method for making optimal use of existing pumping and observation wells for pumping tests [4,5,8,14–17,37,38,65] and cross-hole slug tests [9–11]. The basic idea is to use as many wells as possible for pumping or slug-testing, recording the response in all surrounding wells, and inverting the complete data set to obtain the spatial distribution of hydraulic conductivity, which typically requires regularization. Similarly, tomographic setups for tracer tests have been studied [25,26,63,66,68], but to the best of our knowledge, field applications have not yet been performed, which may be attributed to the associated high experimental effort.

The purpose of this paper is to study the usefulness of thermal arrival-time data obtained in tomographic heat-tracer tests for the assessment of hydraulic conductivity and compare it to the usefulness of head measurements from hydraulic tomography. For simplification reasons we will consider only steady-state hydraulic tomography in combination with mean arrival time measurements of a heat signal obtained from tomographic thermal tracer tests. For both hydraulic and heat-tracer tomography we restrict the analysis to realistic cases in which only few boreholes are large enough to allow pumping.

Because this study is aimed at guiding practical field tests, we choose well setups that account for problems of real field applications. In particular, we consider a nested approach of two injection and two extraction wells, creating a stable (artificial) ambient flow field using the outer well pair and a nested investigation zone using the inner well pair, in which the tracer test is applied [40], to overcome uncertainties in boundary conditions like an unknown ambient flow direction. This scheme has the additional advantage that leakage of the tracer into the environment can be minimized. We restrict the analysis to setups with eight pumping wells in total, because we doubt that any larger number would be affordable in real field investigations. The number of observation points arranged in perpendicular observation planes, in contrast, is much higher. The synthetic test case presented resembles field investigations which are currently performed at the site, and thus the study also aims at guiding the experiments. The well setup and the geometry of the three-dimensional domain is chosen to be as realistic as possible in order to test the quality of inversion results that may be obtainable under realistic, yet optimistic conditions. In contrast to real field studies, the true distribution of parameters is known so that a quantitative statistical analysis of the accuracy of the estimate and its uncertainty is possible.

2. Governing equations and numerical methods

2.1. Forward problem

We assume a locally isotropic hydraulic conductivity field $K(\mathbf{x})$ (m/s) in which $\mathbf{x}$ (m) is the vector of spatial coordinates. The steady-state hydraulic head field $h(\mathbf{x})$ (m) is obtained by solving the groundwater flow equation:

$$-\nabla \cdot (K\nabla h) = Q, \tag{1}$$

subject to the boundary conditions:

$$h = h_0 \text{ at } \quad \Gamma_{\mathrm{D}_h}, \tag{2}$$

$$-\mathbf{n} \cdot (K\nabla h) = q_0 \quad \text{at } \Gamma_{\mathrm{N}_h}, \tag{3}$$

in which $Q(\mathbf{x})$ (s^{-1}) is the volumetric source density, mainly representing wells, Γ_{D_h} denotes a Dirichlet boundary for hydraulic head, h_0 (m) is the corresponding fixed head, $\mathbf{n}$ (m) denotes the unit vector (pointing outwards) normal to the Neumann boundary Γ_{N_h} for hydraulic head, and q_0 (m/s) is a fixed normal volumetric flux at Γ_{N_h}.

The specific discharge $\mathbf{q}$ (m/s) follows Darcy's law:

$$\mathbf{q} = -K\nabla h. \tag{4}$$

and transient heat transport is described by the convection–dispersion equation:

$$\frac{\rho_m c_m}{\rho_w c_w}\frac{\partial T_s}{\partial t} + \mathbf{q}\cdot\nabla T_s - \nabla\cdot\left(\frac{\rho_m c_m}{\rho_w c_w}\mathbf{D}_{T_s}\nabla T_s\right) = Q_{in}(T_{in} - T_s), \tag{5}$$

subject to:

$$T_s(t) = \hat{T}_0(t) \quad \text{on } \Gamma_{\mathrm{D}_T}, \tag{6}$$

$$\mathbf{n}\cdot\left(\mathbf{q}T_s - \frac{\rho_m c_m}{\rho_w c_w}\mathbf{D}_{T_s}\nabla T_s\right) = \hat{q}_{T_s}(t) \quad \text{on } \Gamma_{\mathrm{in}}, \tag{7}$$

$$\mathbf{n}\cdot\left(\frac{\rho_m c_m}{\rho_w c_w}\mathbf{D}_{T_s}\nabla T_s\right) = 0 \quad \text{on } \Gamma\setminus\Gamma_{\mathrm{D}_T}\setminus\Gamma_{\mathrm{in}}, \tag{8}$$

in which t (s) denotes time, T_s (K) is the temperature signal, that is, the deviation from the natural temperature, which is assumed to be constant of the time and space within the experiment. $\rho_w c_w$ (J/K/m^3) and $\rho_m c_m$ (J/K/m^3) are the volumetric heat capacities of water and the bulk porous medium, respectively. $\mathbf{D}_{T_s}$ (m^2/s) is the dispersion tensor of conductive/dispersive heat transfer, $Q_{in} = (Q + |Q|)/2$ (1/s) is the incoming fraction of the volumetric