Evaluation of longitudinal dispersivity estimates from forced-gradient tracer tests in heterogeneous aquifers

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Abstract Converging radial-flow and two-well tracer tests are simulated in two-dimensional aquifers to investigate the effects of heterogeneity and forced-gradient test configuration on longitudinal dispersivity ($\alpha_L$) estimates, and to compare $\alpha_L$ estimates from forced-gradient tests with $\alpha_L$ values that characterize solute spreading under natural-gradient flow. Results indicate that in both mildly and highly heterogeneous aquifers, $\alpha_L$ estimates from two-well tests are generally larger than those from radial-flow tests. In mildly heterogeneous aquifers, $\alpha_L$ estimates from two-well tests with relatively large tracer transport distances are similar to $\alpha_L$ values from natural-gradient simulations. In highly heterogeneous aquifers, $\alpha_L$ estimates from two-well tests at all tracer transport distances are typically smaller than $\alpha_L$ values from natural-gradient simulations.

Key words dispersivity; heterogeneity; numerical modelling; tracer tests

INTRODUCTION

Forced-gradient tracer tests are commonly conducted to estimate the effective porosity and dispersivity of aquifers. When estimating dispersivities by such tests, the typical goal is to obtain values that can be used to characterize solute spreading under natural-gradient conditions. Previous research has addressed some issues related to this objective. Chao et al. (2000) evaluated the effect of heterogeneity on longitudinal dispersivity estimates from converging radial-flow tracer tests and found that in highly heterogeneous aquifers, the estimates typically underestimate those representative of natural-gradient solute spreading. In this paper, we examine the effects of both heterogeneity and tracer test configuration on dispersivity estimates from forced-gradient tests. We numerically simulate different types of forced-gradient tracer tests in aquifers with different degrees of very detailed known heterogeneity, and estimate longitudinal dispersivities from the breakthrough curves. These estimated dispersivities would produce an equivalent degree of tracer spreading if used to simulate a forced-gradient test in an aquifer represented as homogeneous due to lack of knowledge about the heterogeneity. The dispersivity estimates are compared to large-scale dispersivities determined from simulations of natural-gradient tracer transport in the heterogeneous aquifers. These simulations and comparisons are aimed at assessing the applicability of dispersivities estimated from forced-gradient tracer tests for characterizing solute spreading under a natural-gradient flow field.

We present results for converging radial-flow and two-well (dipole) forced-gradient tracer tests, two test types commonly performed to obtain field estimates of
dispersivities. In a converging radial-flow tracer test, a steady flow field is established by pumping water at a constant rate from one well, and a pulse of tracer is quickly injected into a nearby well. In a two-well tracer test, a steady flow field is established by injecting water into one well at a constant rate and pumping water at the same rate from a second well, and a pulse of tracer is added to the injection water.

NUMERICAL SIMULATIONS

Simulation of groundwater flow and representation of hydraulic conductivity

Tracer movement is simulated by first solving for the steady flow field using MODFLOW-96 (Harbaugh & McDonald, 1996). The simulation domain is a horizontal, two-dimensional, square region that is 708.1 m × 708.1 m (Fig. 1). The finite-difference grid has variable spacing, with a finely discretized inner region and a coarsely discretized outer region. The inner region is represented by 1001 rows and 1001 columns, with uniform cell sizes of 0.1 m × 0.1 m. Cell size in the outer region increases with distance towards the outer edge of the domain. The boundary condition at the outer edge is constant head for the radial-flow tests, and is no flow for the two-well tests. For the natural-gradient tracer simulations, constant head boundaries of 1 m and 0 m are specified in, respectively, the first and last columns of the model, and no-flow boundaries are specified on the outer edges of the first and last model rows.

Fig. 1 Simulation domain. Filled circles represent pumped well locations and open circles represent tracer source locations.
The forced-gradient tracer tests are simulated using four different separation distances $R$ (8, 16, 32 and 64 m) between the tracer source location and the pumped well. For the tests with the three smallest values of $R$, the pumped well is at the centre of the simulation domain and the source location is to the left of the pumped well (Fig. 1). For the tests with $R = 64$ m, the pumped well is 18 m from the right edge of the inner grid and the source location is 18 m from the left edge of the inner grid (Fig. 1). For all tracer test simulations, the pumping rate is $1.5 \times 10^4$ m$^3$ s$^{-1}$. For the two-well tests, the injection rate (at the tracer source location) is equal to the pumping rate. The radial-flow tests do not involve simulation of fluid injection.

The hydraulic conductivity ($K$) is heterogeneous in the inner region of the domain, where tracer transport is simulated. A sequential Gaussian simulation procedure (Deutsch & Journel, 1998, p.144, p.170) is used to generate heterogeneous hydraulic conductivity fields, by assuming that $\ln(K)$ is a random function characterized by a spherical variogram $\gamma$ (Deutsch & Journel, 1998, p.25):

$$\gamma(h) = \begin{cases} 1.5 \left( \frac{h}{a} \right) - 0.5 \left( \frac{h}{a} \right)^2 & \text{if } h \leq a \\ c & \text{if } h \geq a \end{cases}$$

where $h$ is separation distance; $c$ is the sill, which is equal to the variance of $\ln(K)$ ($\sigma_{\ln(K)}^2$); and $a$ is the range, which can be considered as a correlation length. In this work, $a$ is set to 0.4 m, which is the distance across four model cells in the inner region.

The mean of the $\ln(K)$ random function is chosen so that the geometric mean of $K$ is $10^4$ m s$^{-1}$. Two values of $\sigma_{\ln(K)}^2$ are used (1.0 and 6.0), to investigate how the degree of heterogeneity affects the longitudinal dispersivity estimates. Twenty $K$ fields are generated for each of these values of $\sigma_{\ln(K)}^2$. In the outer region, $K$ is set to a uniform value of $10^4$ m s$^{-1}$. By considering two different types of forced-gradient tests, four different separation distances, and 20 $K$ realizations for each of the two $\sigma_{\ln(K)}^2$ values, a total of 320 forced-gradient tracer tests are simulated. Natural-gradient tracer migration is simulated in the 20 $K$ fields generated for each of the two values of $\sigma_{\ln(K)}^2$.

**Simulation of solute transport**

Following determination of the steady flow field, tracer transport is simulated by a random walk method that is implemented using a modified version of the particle tracking code MODPATH (Pollock, 1994). A uniform porosity of 0.3 is specified for all cells in the simulation domain. Each simulation is divided into many small transport time steps. During each time step, advective particle movement is calculated using MODPATH. Next, a velocity correction is implemented to ensure that for simultaneous movement of a large number of particles, their density function is consistent with the advection–dispersion equation (Zheng & Bennett, 2002, p.206). Finally, to simulate local dispersion, each particle is randomly displaced in the longitudinal and transverse directions relative to the flow path. The random
longitudinal displacement is $d_L = z_L \sqrt{2a_L \nu \Delta t}$ and the random transverse displacement is $d_T = z_T \sqrt{2a_T \nu \Delta t}$, where $z_L$ and $z_T$ are independent random values from a normal distribution with zero mean and unit variance, $a_L$ is the local longitudinal dispersivity, $a_T$ is the local transverse dispersivity, $\nu$ is the particle velocity, and $\Delta t$ is the transport time step (Zheng & Bennett, 2002, p.205). For all tracer simulations, $a_L$ is set to 0.008 m and $a_T$ is set to 0.0008 m. These local dispersivities represent dispersion processes at scales smaller than a model cell, and were chosen to be very small compared to all separation distances $R$ used in this work.

At the start of each forced-gradient transport simulation, tracer is introduced into the steady flow field by placing a large number of particles in the model cell that represents the tracer source location (the “tracer source cell”). For the converging radial-flow tracer tests, with no fluid injection at the source location, a square array of uniformly-spaced particles is placed within the tracer source cell to represent an instantaneous point input of tracer. Tests with $R = 8$ m use 90 000 particles (an array of $300 \times 300$ particles), and tests with $R = 16, 32$ and 64 m use 160 000 particles (an array of $400 \times 400$ particles). For the two-well tracer tests, particles are placed on the four sides of the tracer source cell in proportion to the groundwater flow rate across each side, to approximate an instantaneous pulse input of tracer into the injection water. Tests with $R = 8$ m use 200 000 particles and tests with $R = 16, 32$ and 64 m use 400 000 particles. The random walk method simulates movement of the particles placed in the tracer source cell through the steady flow field. The particle arrival times at the pumped well are recorded, and a histogram is constructed by dividing the simulation into uniform time increments and counting the number of particles that arrive within each increment. The histograms are converted to concentration breakthrough curves by normalizing by the total number of particles, and assuming an initial concentration in the tracer source cell.

At the start of each natural-gradient transport simulation, a rectangular array of 50 100 particles is placed near the left edge of the inner region of the simulation domain (Fig. 1). This array spans 501 model cells that occupy one model column and 501 model rows. Each of the 501 cells contains 100 particles configured as a square array of $10 \times 10$ particles. Particles are placed only in the central half of the rows in the inner region so that as they spread laterally while migrating downgradient, they remain in the heterogeneous part of the domain. At several simulation times, the number of particles in each model cell is recorded, and these particle positions are used to calculate the second spatial moment of the particle plume, as described below. The simulation is terminated when the particle that travels fastest across the inner region reaches the downgradient boundary of the inner region.

**ESTIMATING LONGITUDINAL DISPERSIVITY**

Values of longitudinal dispersivity ($\alpha_L$) are estimated for the simulated forced-gradient tracer tests by analysing the breakthrough curves with type curves constructed from solutions to the advection–dispersion equation derived for homogeneous media. Each type curve is characterized by a unique Peclet number, $Pe = R/\alpha_L$. For the converging radial-flow tests, the analytical solution derived by Moench (1989, 1991) is used. For
the two-well tests, the solution for homogeneous media is derived using a random walk method similar to that described above, except that advective particle movement is simulated using an analytical expression for the velocity. This approach produces a solution that is more accurate for small Peclet numbers than the approximate solution of Welty & Gelhar (1994).

Each simulated breakthrough curve is analysed by manually matching its rising limb and peak to the corresponding parts of a particular type curve. The estimated value of \( \alpha_L \) for the simulated tracer test is then computed from the Peclet number that characterizes the type curve. Manual curve matching was considered the best approach for estimating an effective \( \alpha_L \) value, because the simulated breakthrough curves are typically choppy, and can have more than one peak. We fit only the rising limb and peak because commonly, the entire simulated breakthrough curve cannot be fit to a single type curve. Matching only the rising limb and peak appears to be a standard method for estimating \( \alpha_L \) from forced-gradient tracer tests, as illustrated in the case studies presented by Welty & Gelhar (1994).

For each natural-gradient tracer simulation, a large-scale \( \alpha_L \) is determined using spatial moment analysis of the tracer plume (Freyberg, 1986). First, the second spatial moment about the centre of mass in the longitudinal direction (along model rows) is determined at several times. The longitudinal variance \( \sigma_L^2 \) of the plume is then computed from the second moment. The large-scale \( \alpha_L \) that characterizes the tracer spreading is a function of the temporal rate of change of \( \sigma_L \): \( \alpha_L = (1/[2\bar{v}]) (d\sigma_L/dt) \), where \( \bar{v} \) is the mean particle velocity across the inner region. At the end of the natural gradient simulations for \( \sigma_{Ln}^2(K) \) equal to both 1.0 and 6.0, \( d\sigma_L/dt \) becomes nearly constant, and thus \( \alpha_L \) reaches a nearly asymptotic value.

RESULTS AND DISCUSSION

The \( \alpha_L \) estimates from all forced-gradient tracer tests and natural-gradient tracer simulations are summarized in Fig. 2. Comparison of the results among the two types of forced-gradient tracer tests suggests that for all separation distances, in both the mildly \( \sigma_{Lm}^2(K) = 1.0 \) and strongly \( \sigma_{Ls}^2(K) = 6.0 \) heterogeneous aquifers, the \( \alpha_L \) values determined from the two-well tests are generally larger than those from the radial-flow tests.

The degree to which the \( \alpha_L \) estimates from the forced-gradient tests approximate the estimates from the natural-gradient simulations depends on both the level of heterogeneity and the separation distance. For \( \sigma_{Lm}^2(K) = 1.0 \) and larger values of \( R \), the \( \alpha_L \) estimates from the two-well tests are similar to those from the natural-gradient simulations, but the \( \alpha_L \) estimates from the radial-flow tests are smaller than those from the natural-gradient simulations (Fig. 2). For \( \sigma_{Ls}^2(K) = 6.0 \), at the largest separation distance considered, both the radial-flow and two-well tests yield \( \alpha_L \) estimates that are considerably smaller than the natural-gradient \( \alpha_L \) estimates. However, the \( \alpha_L \) estimates from the two-well tests are clearly closer to the natural-gradient \( \alpha_L \) values. The results thus suggest that for highly heterogeneous aquifers, a two-well test is more likely than a radial-flow test to yield a \( \alpha_L \) estimate that characterizes natural-gradient solute spreading.
Consideration of the aquifer volume sampled by the tracer during different forced-gradient test configurations provides insight into the results of this work. In a converging radial-flow test, the tracer samples a relatively narrow volume of aquifer between the source location and the pumped well. In contrast, during a two-well test, the tracer samples a significantly larger volume, because injected water at the source location spreads the tracer into a wider region between the source and the pumped well. As the separation distance \( R \) increases, the volume sampled by the tracer during a two-well test becomes increasingly larger than that sampled during a radial-flow test. This observation, together with the finding that for large \( \sigma_{ln(K)}^2 \) and large \( R \) the two-well tests yield \( \alpha_L \) estimates that are closest to the \( \alpha_L \) values determined for the natural-gradient simulations, leads to the following preliminary conclusion. It is important that a large aquifer volume be sampled by the tracer during a forced-gradient test, to increase the likelihood that the \( \alpha_L \) estimate from the test will be representative of solute spreading under natural-gradient conditions.

REFERENCES


