Estimating lithologic and transport properties in three dimensions using seismic and tracer data: The Kesterson aquifer

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Abstract. The identification of aquifer heterogeneities, particularly flow paths and barriers, has become a critical research topic in hydrogeology. Cross-well seismic tomography may provide the needed resolution when used in conjunction with hydraulic head and tracer concentration measurements. We demonstrate a field application and sensitivity analysis of the split inversion method (SIM), which combines seismic, hydraulic, and tracer data to estimate the three-dimensional zonation of aquifer properties along with the hydraulic properties for these zones. For the Kesterson aquifer in the San Joaquin Valley, California, we first invert seismic travel times measured between six well pairs to obtain seismic slowness (1/seismic velocity) cross sections, or tomograms. We then use conditional simulation to provide three-dimensional seismic slowness realizations. Next, the SIM is used to split several realizations into three lithologic zones and assign hydraulic properties to the zones to best match six tracer concentration histories.

Introduction

Spatial variability of hydraulic conductivity provides a predominant control on groundwater flow and solute transport. Hydraulic conductivity commonly varies over several orders of magnitude for different lithologies, and aquifers generally exhibit complex lithologic patterns. Thus accurate conductivity estimates are needed to predict the fate of contaminants in aquifers and to efficiently design remedial schemes for contaminated sites.

Hydraulic conductivity values are typically derived from a small number of pumping tests and laboratory core measurements [Yeh, 1986]. At highly heterogeneous sites these data are inadequate to fully describe the conductivity variations. A common approach is to parameterize the domain into homogenous zones and assign a hydraulic parameter to each zone [Cooley, 1977, 1979]. However, there are rarely enough data to uniquely parameterize a region into meaningful zones and determine the conductivity value for each zone [Yeh, 1986].

A potential solution to this problem is to use densely sampled geophysical information to help parameterize zones and values. Geophysical methods, such as cross-well seismic tomography, can be used to infer the pattern of lithologies between wells. Cross-well seismic tomography is the process of inverting seismic travel times for a seismic slowness (1/seismic velocity) image between wells. It is similar in philosophy to the computed axial tomography (CAT) scan used in medical imaging [Dines and Lyle, 1979], however, in this case one is using sound waves to image subsurface geology rather than X rays to image the human body. Seismic tomography has been employed to successfully characterize petroleum reservoirs but has rarely been used to characterize shallow aquifers.

Several authors have indicated that seismic information can be used to infer the hydrogeologic properties of aquifers and reservoirs. Araktingi and Bashore [1992] explored the effect of adding three-dimensional surface seismic data to well log data for petroleum reservoir characterization. McKenna and Poeter [1995] classified, on the basis of both hard and soft data, the hydrofacies of a site using discriminant analysis. Copty and Rubin [1995] presented a stochastic method that combines surface seismic data and lithologic logs to identify subsurface lithologies. Doyen et al. [1991] estimated lithologies from seismic data and lithologic observations in wells using a Monte Carlo approach. Rubin et al. [1992] developed an approach to invert pore pressure data for a permeability field, given perfect knowledge of the seismic velocity field and a known relation between seismic velocity and permeability. This method was then extended by Copty et al. [1993] to estimate the spatial distribution of permeability given a seismic velocity field with spatially uncorrelated errors. Some of these methods are limited by their reliance on knowledge of the relation between seismic velocity and the hydrogeologic properties (lithology or permeability), which is generally unknown at the field scale.

To address this limitation, Hyndman et al. [1994] introduced the theoretical concept of the split inversion method (SIM) that does not rely on knowledge of the relationship between seismic velocity and hydraulic conductivity. The SIM inverts seismic travel times and tracer concentration histories for the zonation of lithologies, hydraulic conductivity values for each zone, and the value of dispersivity for the region. The motivation for the SIM is that seismic energy and tracer concentrations each have independently sampled regions of the same physical environment. Their combined analysis should improve the description of this environment relative to estimates made with either data set alone. Cross-well seismic travel times provide densely sampled spatial information along vertical planes between wells, which complements the spatially averaged three-dimensional information from pumping tests and tracer tests. Hyndman et al. [1994] demonstrated the SIM for two synthetic sandy aquifers, one with embedded clay zones and...
Hyndman et al. [1994] to the case of three dimensions with three unique zonal lithologic classes and applies the approach to a field site.

Hydrogeologic Setting

Several regional groundwater studies have been completed in the San Joaquin Valley, California, owing to the importance of the region’s agriculture [National Research Council, 1993]. The U.S. Geological Survey conducted a regional study in the San Joaquin Valley to evaluate the aquifer system, identify changes due to development, and simulate past and present conditions [Williamson et al., 1989]. Belitz et al. [1993] and Belitz and Phillips [1995] then developed a three-dimensional groundwater flow model of the central part of the western San Joaquin Valley to assess alternatives to agricultural drains for managing the water table elevation. These studies offer some insight into the aquifer characteristics.

The shallow aquifer below Kesterson Reservoir, which is located in the San Joaquin Valley, was contaminated with agricultural return water during the 6-year operation of the reservoir ending in 1986. Regional collector drains were installed in the western part of the valley in the early 1980s to prevent reduced agricultural production due to shallow saline water. This saline water was pumped from the collector drains to Kesterson Reservoir, where approximately 50% of the water seeped into the ground [Benson et al., 1991].

The Kesterson site received public attention when a high rate of deformities was found in the embryos of waterfowl that nest in the Kesterson region. These deformities were linked to high selenium concentrations in the water discharged from drains into Kesterson Reservoir. The naturally occurring selenium leached from the irrigated farmlands of the San Joaquin Valley [Ohlendorf et al., 1986].

The sediments of the shallow, semiconfined Kesterson aquifer were deposited by the San Joaquin River, which meanders through the valley depositing sand and silt from the Sierra Nevada. These sediments are stratigraphically above and thus younger than the Corcoran clay, which is approximately 620,000 years old [Dalrymple, 1980]. The Corcoran clay, which is the major confining layer for the deeper aquifers, is approximately 75 m deep in the San Joaquin Valley trough [Hotchkiss and Balding, 1971]. Widespread lacustrine clay deposits such as the Corcoran are present at several depths throughout the valley. One of these clays, at approximately 20 m depth, separates the aquifer that is the focus of our study from the deeper semiconfined aquifer [Benson, 1988]. The saturated thickness of the shallow aquifer is approximately 19 m since the water table at the Kesterson site was approximately 1 m deep in 1985 [Benson, 1988].

We use three data sets to estimate the heterogeneous hydraulic properties of the shallow Kesterson aquifer: tracer concentration histories, seismic travel times, and drawdown. A multiple-well fluorescein tracer test was conducted in the shallow Kesterson aquifer by Benson [1988] to predict the movement of the selenium plume and determine the nature of heterogeneities at the site. Drawdown was measured in an observation well during this tracer test. In addition, seismic travel times were collected between six well pairs that cover the central portion of the tracer test (E. Majer, personal communication, 1994). Figure 1 is a map of the Kesterson aquifer, with lines connecting the well pairs used in the seismic test and open circles denoting the locations of the tracer measurement wells. The well screens were located at different depths (Table 1) to provide sensitivity to hydraulic conductivity with depth. Unfortunately, no well logs were available to compare the lithologies to the seismic and hydraulic property estimates at this site.

In the remainder of this paper we demonstrate how these seismic, hydraulic, and tracer data are combined to deduce the lithologic zonation and flow and transport properties of the shallow Kesterson aquifer. First, the seismic travel times for all available well pairs are convolved for two-dimensional slowness tomograms through the aquifer. Geostatistical methods are then used to generate equally likely three-dimensional conditional slowness realizations. Finally, randomly chosen realizations, which are conditioned to the six two-dimensional tomograms, are split into three lithologic populations, and each population is assigned a hydraulic conductivity value to
best match the tracer and hydraulic data. In this approach, seismic travel times provide an estimate of the lithologic structure, while tracer concentrations and drawdown are used to split the seismic estimate into lithologic zones and assign conductivity values to each zone.

### Seismic Inversion

The first stage of this approach to estimate the shallow Kesterson aquifer properties involves imaging the subsurface using seismic tomography. The main goals of this tomographic inversion are to image the main lithologies in the aquifer and to estimate the correlation structure of the aquifer.

The data used for this seismic inversion are the travel times between multiple sources and multiple receivers (provided by E. Majer, Lawrence Berkeley Laboratory, 1994). These travel times are then inverted for seismic slowness cross sections at the site, which are called tomograms. Seismic energy (sound waves) of a predetermined frequency was generated at equal depth intervals (0.3 m) in the source well. There were between 13 and 23 source locations per well. The resulting signal from each source was measured at 12 to 29 receivers (0.3-m interval) in a nearby well. For the Kesterson site the seismic source was a piezoelectric bender bar, and the receivers were hydrophones. Sound waves of specified frequency (6–10 kHz) were generated at the source by controlling an electric current through the piezoelectric material, which expands and contracts in response to this current. The measured signal can be compressed into a few key measures such as travel times and amplitudes, which can then be inverted for geophysical properties. The compressional wave travel times between each source and receiver serve as our data for cross-well seismic tomography, although, as discussed in our conclusions, seismic amplitudes could be inverted for attenuation coefficients that may be correlated to hydraulic properties.

We used an algorithm, called the multiple population inversion (MPI), to invert all the measured Kesterson travel times for the geometry of three slowness populations as discussed by Hyndman and Harris [1996]. The objective of the MPI is to minimize the average absolute travel time residual for all source-receiver pairs. The MPI constrains the slowness field to a specified number of values, which reduces artifacts commonly seen in unconstrained tomographic inversions without smoothing the estimated image. Smoothing is the most common method of reducing artifacts from ray-based tomographic inversions, which reduces the ability of the inversion to resolve small-scale heterogeneities.

The MPI converged to approximately the same objective value as obtained from an unconstrained form of this tomographic inversion, despite the constraint that only three slowness values were allowed for the region [Hyndman and Harris, 1996]. This suggests that three discrete slowness values can be used to describe the predominant heterogeneities at the Kesterson site. The zonal slowness estimate was then used as a starting model for an unconstrained tomographic inversion, which preserved the large-scale structure and added some finer-scale heterogeneities. This was done because unconstrained iterative inversions worked well when the starting model is close to the true slowness field and because the unconstrained estimates can be used to infer the correlation structure of the Kesterson lithologies. These updated slowness tomograms are shown in Plate 1a with a corresponding histogram of the estimated values. The estimated slowness cells are 15 cm on a side, providing high-resolution information about the seismic slowness structure of the aquifer. The size of these cells is controlled by the vertical spacing of sources and receivers (30 cm) and by the wavelength of the seismic signal. The finest resolution possible from a seismic signal is approximately a quarter wavelength (λ), which is calculated using the relation λ = 4/f where f is the frequency of the seismic signal. The finest resolution possible is 15 cm on a side, providing high-resolution information about the seismic slowness structure of the aquifer.

### Extension From Multiple Two-Dimensional Images to Three-Dimensional Images Using Conditional Geostatistics

Although the two-dimensional slowness tomograms provide useful information about the nature of heterogeneity at the site, we would like estimates of the aquifer properties in three dimensions. Full three-dimensional slowness estimates can be

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**Table 1. Kesterson Tracer Well Locations and Hydraulic Conductivities**

<table>
<thead>
<tr>
<th>Well*</th>
<th>X Coordinate, m</th>
<th>Y Coordinate, m</th>
<th>Screened Interval, m</th>
<th>Diameter, m</th>
<th>Hydraulic Conductivity, † m/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>I2</td>
<td>−0.5734</td>
<td>16.1150</td>
<td>6.1–12.2</td>
<td>0.10</td>
<td>2.1 × 10⁻⁴</td>
</tr>
<tr>
<td>ST1</td>
<td>−3.3822</td>
<td>0.9600</td>
<td>6.1–7.6</td>
<td>0.05</td>
<td>6.0 × 10⁻⁴</td>
</tr>
<tr>
<td>ST2</td>
<td>−3.4336</td>
<td>3.3700</td>
<td>7.6–9.1</td>
<td>0.05</td>
<td>5.9 × 10⁻⁴</td>
</tr>
<tr>
<td>ST3</td>
<td>−0.6498</td>
<td>−0.0500</td>
<td>9.1–10.7</td>
<td>0.05</td>
<td>1.6 × 10⁻⁴</td>
</tr>
<tr>
<td>ST4</td>
<td>0.0900</td>
<td>0.0000</td>
<td>10.7–12.2</td>
<td>0.05</td>
<td>2.4 × 10⁻⁴</td>
</tr>
<tr>
<td>ST5</td>
<td>−1.3557</td>
<td>−0.0300</td>
<td>12.2–13.7</td>
<td>0.05</td>
<td>...</td>
</tr>
<tr>
<td>ST8</td>
<td>−1.8284</td>
<td>5.6300</td>
<td>10.7–12.2</td>
<td>0.05</td>
<td>...</td>
</tr>
<tr>
<td>I1</td>
<td>−1.5034</td>
<td>2.3430</td>
<td>6.1–12.2</td>
<td>0.10</td>
<td>3.4 × 10⁻⁴</td>
</tr>
<tr>
<td>ST6</td>
<td>−3.3988</td>
<td>−13.8738</td>
<td>6.1–12.2</td>
<td>0.10</td>
<td>1.4 × 10⁻⁴</td>
</tr>
</tbody>
</table>

* Wells ST1 through ST8 are labeled 1 through 8 in the text and figures for clarity.
† Hydraulic conductivity values were estimated by Benson [1988] using single-well steady state pumping tests.
Plate 1. (a) Three-dimensional layout of seismic slowness estimates at the Kesterson site, in which the red lines represent well locations. Wells 5 and 4 are at the east side of the image, and well I2 is at the west (see Figure 1 for location map). The histogram illustrates the bimodal nature of the slowness estimates at the site. (b) Three-dimensional slowness realization generated using sequential Gaussian simulation, which preserves the correlation lengths and probability distribution from the seismic tomograms and provides a geologically reasonable estimate for the Kesterson site.
extrapolated from the tomograms using geostatistical methods, such as kriging and conditional simulation.

The range of likely correlation parameters for these conditional simulations can be inferred from the tomograms in Plate 1a. Figure 2 illustrates the calculated sample variograms from both a single seismic slowness tomogram (between wells 4 and 8) and a three-dimensional analysis of all the tomograms. The tomogram from well 4 to well 8 was chosen for this analysis because it has many source receiver pairs and approximately 45° of ray coverage. The three-dimensional variogram analysis of the tomograms was conducted after decluster ing the slowness estimates to reduce bias caused by unrepresentative variabil ity at the contact between tomograms. We first estimated the correlation lengths by fitting exponential variograms ($\lambda_h$ = between 5 and 9 m, $\lambda_v$ = 0.9 m, $\sigma^2$ = 104 (calculated population variance)) to these sample variograms (Figure 2). We then generated conditional slowness realizations with a range of correlation lengths and completed the full inversion described below for each realization. We found that realizations generated with a horizontal correlation length of 9 m and a vertical correlation length of 0.9 m resulted in the best fit to the tracer data, as discussed in the sensitivity analysis section. If long tomograms had been available in multiple directions, we also could have inferred the direction and magnitude of the horizontal anisotropy. The estimated sample variance appeared to be isotropic; thus only the correlation lengths changed with direction.

For this study we used sequential Gaussian simulation to generate equally likely slowness realizations that are conditioned on the six estimated seismic slowness planes (tomograms) with different orientations. The steps of this conditional simulation approach are [Deutsch and Journel, 1992] as follows:

1. Transform the distribution of slowness estimates (mean = 574 μs/m, variance = 104) to a standard normal probability distribution (mean = 0.0, variance = 1.0) using a normal scores approach.

2. Generate a random path that visits each node of the three-dimensional grid once.

3. Determine, for each node, the mean and variance of the conditional distribution function using simple kriging of the normally distributed slowness estimates by using an anisotropic search radius (vertical = 0.1 × horizontal). Then draw a simulated slowness value from this conditional distribution. Continue along the random path until all locations are simulated.

4. Back transform the normally distributed three-dimensional estimates to the original distribution of slowness estimates (mean = 574 μs/m, variance = 104), using the reverse of the transform used in step 1.

Each simulated value is thus a weighted average of the slowness estimates and previously simulated points, with the weights resulting from the kriging equations based on the estimated horizontal and vertical variograms (Figure 2). Each realization from this method preserves the seismic slowness values along the six tomographic planes (Plate 1a) and the horizontal and vertical correlation structure from the specified variograms. This approach also preserves the probability distribution of the two-dimensional slowness estimates, as illustrated by the nearly perfect agreement between histograms in Plate 1a and 1b.

Plate 1b illustrates a randomly chosen slowness realization generated with an exponential variogram ($\lambda_h$ = 9 m, $\lambda_v$ = 0.9 m, $\sigma^2$ = 104) for the Kesterson aquifer. The cell size for these realizations is 1.5 m on a side and 0.4 m vertically, which preserves most of the structure from the tomograms and is a reasonable grid size for solute transport simulation. Plate 1b is illustrated with additional interpolated cells for visual clarity (four times the horizontal cells and two times the vertical cells with linear interpolation).

Each realization preserves the slowness values at locations where we have conditioning slowness estimates from the tomograms, but away from the conditioning points the realizations can differ significantly from one realization to the next. Thus the uncertainty in our three-dimensional slowness estimates is low near the tomograms and high near the edge of each estimated slowness realization.

The next stage of our approach is to include the analysis of the tracer data. The slowness realizations are split into zones using the SIM, and these zones are assigned flow and transport parameters to match the tracer data. In this paper the results are shown for just one slowness realization. The results appear similar for four additional realizations with the same variance and correlation lengths because of the large quantity of conditioning “data” in the region of the tracer test.

**Tracer Inversion**

In July 1986 a multiple-well tracer test with an injection/withdrawal well pair was performed to infer the flow and trans-
port properties of the shallow Kesterson aquifer [Benson, 1988]. The pumping and injection rates were maintained at 4.73 × 10⁻³ m³/s (75 gallons/min) for 24 hours prior to tracer introduction. A 3180-s (53-min) pulse of fluorescein dye was then put into the injection well, providing an inflow concentration of approximately 320 ppm [Benson, 1988]. Fluorescein is a weakly sorbing tracer, as determined by Smart and Laidlaw [1977] using batch experiments with different sediments. Thus for this study we assume that fluorescein is a conservative tracer.

The resulting concentrations were measured at six down gradient wells (see Figure 1 and Table 1 for well locations and screen depths) throughout the following 10 days, during which pumping and injection were maintained at the same rate (4.73 × 10⁻³ m³/s). Each sample from the monitoring wells was taken using a borehole mixing system described by Benson [1988]. This mixing system recirculates fluid through the screened interval for a short period of time then collects a sample for fluorescence analysis. The goal of this mixing approach was to collect a sample that represents the average concentration across the screened interval. These six concentration histories serve as the data to estimate the lithologic zonation and hydraulic properties for each zone.

The SIM [Hyndman et al., 1994] was used to split the three-dimensional slowness realizations into three populations, estimate the hydraulic conductivity for each population, and infer a regional dispersivity value. In other words, the SIM splits the slowness realizations into zones. The lithologies of these zones can then be inferred from the hydraulic property estimates, knowledge of the regional geology, and correlation of the estimates with lithologic logs.

Tracer tests provide information that can be used to infer the flow and transport properties of porous media. The SIM is implemented as a simulation-regression algorithm [Gailey et al., 1991; Wagner and Gorelick, 1987] to best match the measured concentration histories using six physically based parameters. These parameters are two seismic slowness values that split the slowness realizations into zones, three hydraulic conductivity values (one for each slowness zone), and a single longitudinal dispersivity value (assuming αₜ = 0.2 αₑ) for the region (Table 2). Using these parameters, we simulate steady state groundwater flow and nonreactive solute transport through the Kesterson aquifer using a numerical solution of the three-dimensional groundwater flow equation (1), Darcy’s law (2), and the three-dimensional advection-dispersion equation (3):

\[
\nabla \cdot (K \nabla h) = W
\]

\[
v = -\frac{K}{\theta_e} \nabla h
\]

\[
\frac{dc}{dt} + \nabla (v \cdot c) - \nabla \cdot (D \nabla c) = \frac{c'}{\theta_e}
\]

where

- \nabla gradient operator (\(\partial/\partial x, \partial/\partial y, \partial/\partial z\));
- x, y, z Cartesian coordinates [m];
- K hydraulic conductivity [m/s];
- h hydraulic head [m];
- W fluid source sink term (positive for source) [l/s];
- v groundwater velocity vector [m/s];
- \(\theta_e\) effective porosity [-];
- c’ tracer concentration in source or sink [ppm];
- t time [s];
- D hydrodynamic dispersion coefficient, \(D = D(\alpha_e, \alpha_t, v)\) [m²/s]; and
- \(\alpha_e, \alpha_t\) longitudinal and transverse dispersivities [m].

The effective porosity is assumed to be homogeneous at 30% [Lawrence Berkeley Laboratory (LBL), 1986; Liu and Narasimhan, 1994], which is reasonable since porosity is known to vary over a much smaller range than hydraulic conductivity. The tracer velocity scales proportionally to hydraulic conductivity divided by effective porosity according to Darcy’s law (2); thus the quantity conductivity over effective porosity is the parameter we are estimating using tracer data. If the assumed effective porosity is incorrect, the hydraulic conductivity estimates should be scaled by the ratio true porosity/assumed porosity. If adequate head data were available, both the conductivities and effective porosities could perhaps be simultaneously estimated.

The objective of the SIM was to minimize the sum of squared residuals between measured and simulated tracer concentration arrival time quantiles at the six measurement wells and drawdown at well HO60 (4) for each of the five realizations. The zonation of the slowness image and the hydraulic conductivity values are adjusted to minimize this objective value. Each tracer concentration history was represented using nine quantiles. Each quantile represents the time at which a specified percent (e.g., 10%, 20%, ..., 90%) of the measured tracer mass passes the observation well.

\[
\text{min } R = \left[ \sum_{w} \sum_{i=1}^{9} \left( \frac{\tau_{i,\text{meas}} - \tau_{i,\text{sim}}}{\tau_{i,\text{meas}}} \right)^2 + \beta \left[ (\Delta h_{\text{meas}} - \Delta h_{\text{sim}})^2 \right] \right] \]

where

- \(R\) sum of squared residuals [days²];
- \(\tau_{i,\text{meas}}\) i⁰ₘᵢₐᵢₜ measured concentration arrival time quantile for well w [days];
- \(\tau_{i,\text{sim}}\) i⁰ₕᵢₜ simulated concentration arrival time quantile for well w [days];
- \(\beta\) weight to provide sensitivity to both tracer and drawdown data [(days/m)²];
- \(\Delta h_{\text{meas}}\) measured drawdown at well HO60 (see Figure 1 for location) [m]; and
- \(\Delta h_{\text{sim}}\) simulated drawdown at well HO60 [m].

The weighting factor (\(\beta\)) can be adjusted to normalize the contribution of different data sets. In all cases there is an implicit weight because of the specified units for the two data sets. For example, if the drawdown were measured in centimeters, the squared drawdown residuals would have an implicit weight 10,000 times larger than if drawdown were measured in meters, without changing the units on the concentration arrival time quantiles. In this case a weight of 1076 provided sufficient sensitivity to both the hydraulic and tracer data. Several weights were used in a range covering an order of magnitude about this value, and the estimated values changed by less than 1%. Drawdown was most sensitive to the mean conductivity while the concentration histories were most sensitive to the difference in conductivities between zones.

MODFLOW, which is the U.S. Geological Survey’s three-
dimensional groundwater flow model [McDonald and Harbaugh, 1988], was used to solve (1) for the hydraulic head field using a zonal estimate of the hydraulic conductivity field and appropriate boundary conditions (no flow through bottom and constant head of 14.6 m on all sides, based on head measurements by Benson [1988]; ground surface is at 15.25 m). The Kesterson aquifer grid was 37 cells in the east-west direction, 35 cells in the north-south direction, and 32 cells in the vertical direction. Each cell was 1.5 m on a side and 0.4 m vertically. We modified the MODFLOW code to automatically calculate the vertical hydraulic conductivity based on the specified horizontal conductivity field, assuming no anisotropy. We assume that flow and transport through this aquifer can be described using isotropic hydraulic conductivity values at the scale of an estimated zone. Anisotropy at subzonal scales would be justified if laboratory or field tests indicated significant differences in horizontal and vertical flow rates. Large-scale anisotropy effects can be captured by resolving the heterogeneous structure of the aquifer with our characterization approach. This approach could easily include anisotropy coefficients for each zone if tracer data were measured with a resolution finer than that at the Kesterson site. We also adapted MODFLOW to automatically distribute the total well flow rates in proportion to the hydraulic conductivity of each screened grid cell.

MT3D [Zheng, 1992] was used for the tracer simulations because the method of characteristics approach employed in this model is an efficient and effective method to calculate concentrations through time for advectively dominated systems [Zheng, 1993] such as the Kesterson aquifer. Computational efficiency is especially important for simulation-regression algorithms because large numbers of forward simulations are needed to obtain accurate parameter estimates. The grid used for the MT3D simulations was the same as that used in the MODFLOW simulations.

MT3D first calculates the groundwater velocities using Darcy's law (2) and the hydraulic head field from MODFLOW. Then it tracks particles as they move through the predicted velocity field. At the end of each time step the dispersion term of (3) is calculated using a finite difference approach. Thus MT3D uses a mixed Eulerian-Lagrangian approach to calculate tracer concentrations for each time step. For each observation well, we calculated the vertical flux average of the calculated grid cell concentrations through the screened interval (weighted proportional to the estimated hydraulic conductivity at each depth) [Parker and Van Genuchten, 1984]. The regression code then compares the simulated and observed tracer quantiles at the six measurement wells and the drawdown at well HO60 and minimizes the objective value (4) for each realization.

Results

Figure 3 illustrates tracer simulations and the resulting concentration histories for the estimated parameters listed in Table 2 and the slowness realization illustrated in Plate 1b. The specified slowness splits result in the zonation of hydraulic conductivity illustrated in Figure 4. The region is modeled using the rectangular cells from the conditional slowness realizations, with specified head boundaries on all four sides of the region pictured in Plate 1b. No regional gradient was apparent in head maps presented by Benson [1988]; thus no regional gradient was included in this model. The bottom of the region was considered to be a no-flow boundary, since a clay is present at a depth of approximately 20 m in wells throughout the Kesterson region [Benson, 1988]. The first 4 m of the aquifer below the ground surface (i.e., the interval overlying the conditional simulation) was described as a fine grained surficial layer by Benson et al. [1991], and were thus modeled as low conductivity cells (3.5 × 10−6 m/s, as determined by Luthin [1966]). All the inflow boundaries were specified as zero-concentration cells. The effect of these boundary conditions was reduced by placing the boundaries far from the injection and withdrawal locations.

Simulated concentration profiles obtained using the parameter estimates in Table 2 are illustrated in Figure 3a. The injection well is located approximately in the center of the tracer plume in Figure 3a, and the pumping well is approximately at the center of the white arrow. Groundwater is flowing in the direction of the arrow, from the injection well to the pumping well. Two days after the tracer injection, the simulated concentration front of 1 ppm (white isocontour in Figure 3a) appears to be fairly spherical around the injection location. At 8 days the effects of the heterogeneous hydraulic conductivity field are apparent as the tracer has moved more rapidly toward the withdrawal well in the white near-surface highconductivity zone than in the black low-conductivity zone at depth (Figure 4). The hydraulic conductivity values were determined by inverting the tracer data rather than inferring these properties directly from the seismic estimates because the relationship between slowness and conductivity is unknown. The heterogeneity in the conductivity field results in significant variability in the simulated concentration histories at the measurement wells.

The vertically averaged concentrations illustrated in Figure 3b do not reflect the degree of heterogeneity at the site because most of the conductivity variability is in the vertical direction. Figure 3c shows the match between measured and simulated (using parameters in Table 2) tracer concentration arrival histories at well H1, which is screened through most of the simulated aquifer thickness. This illustrates that the vertically averaged concentrations are fairly representative of the measured concentrations for a well with a long screen, but we either need wells at multiple depths or multilevel samplers to fully assess the vertical heterogeneity at this site.

The estimated parameters in Table 2 and zonation illustrated in Figure 4 result in a reasonable match of most of the concentration histories, as illustrated in Figure 5. The central tendency and main peaks of the concentration histories are matched at all measurement wells, with the possible exception of wells 3 and 8. A significant difference is the relative smoothness of the simulated concentration histories relative to the measured concentration histories. This is likely a result of small-scale heterogeneities that either were not imaged with our approach or were outside of the area of dense seismic tomograms. It is also possible that zones of similar seismic slowness have different hydraulic properties, in which case we require some additional information (e.g., more detailed tracer measurements in space or estimates of seismic attenuation coefficient) to accurately estimate the hydraulic conductivity of these zones. Although the presented method was developed to handle nonunique relations between slowness and log conductivity [Hyndman et al., 1994], we assumed that an estimated slowness zone had a single value of hydraulic conductivity at Kesterson because of the limited hydraulic and tracer data. In addition, many of the measured peaks are very sharp and thus difficult to accurately simulate. These results illustrate that seismic and tracer data can be combined to generate estimates.
of subsurface lithologic zonation and determine the flow and transport properties for each zone that are consistent with all available data.

The tracer inversion begins with an initial guess of the parameters and adjusts these parameters to minimize the objective value (4) using a gradient search. We employed multiple line searches in the direction of each parameter because of the highly nonlinear nature of this inversion. For each parameter a line search is used to find the minimum objective value to a predetermined convergence criteria [Press et al., 1989]. Each parameter's line search first brackets the minimum, and then uses parabolic interpolation to converge toward the optimal parameter value. After a line search is completed on each parameter, all parameters are updated on the basis of the calculated gradient of the objective function. This approach does not find a local minima if the step size for parameter adjustment is large. As the inversion proceeds the step size can be reduced to obtain a slightly improved objective value. Although this nonlinear estimation approach worked well for this field case, different techniques can be used depending on the nature of the objective function. For this case the need to escape from local minima was critical to the success of the inversion; thus the step size determination was important.

Starting at different initial parameter values is useful to determine if the estimates are at a local minima. Since this is a highly nonlinear inversion, multiple starting points were used to determine if the parameter estimates provide a global optimum or if the problem is nonunique. If the starting values are far from optimal, convergence may be slow, or the method may converge to one of the local minima. Thus the first stage of the inversion is to bracket the parameter values to put the concentration peaks in roughly the correct places using forward simulations. Then the inversion is used to adjust the values to obtain the best fit to the measurements.

Figure 3. (a) Three-dimensional simulations of solute transport are used to match the tracer concentration histories at each measurement well. (b) The vertically averaged concentrations are shown with the location of well I1, which has a long screened interval and thus approximately samples the vertically averaged concentration. (c) The values of slowness splits and hydraulic conductivity are adjusted to minimize the difference between the measured and simulated concentration histories.
The range of hydraulic conductivity values that we found was from $1.4 \times 10^{-4}$ m/s to $5.0 \times 10^{-4}$ m/s (Table 2), which compares favorably to previous estimates from this area. Conductivities in the range of $1.4 \times 10^{-4}$ to $6.4 \times 10^{-4}$ m/s (Table 2) were reported for pumping tests at the HO site, where the multiple well tracer test was completed [Benson, 1988; Benson et al., 1991]. Benson [1988] also reported conductivities in the range of $8.8 \times 10^{-5}$ m/s to $1.1 \times 10^{-3}$ m/s for 20 single-well pumping tests from the shallow Kesterson aquifer.

Benson [1988] interpreted the tracer concentration histories using the superposition of many one-dimensional advection dispersion solutions. With this approach Benson [1988] estimated the thickness, flow velocity, and dispersivity for multiple one-dimensional paths to each tracer measurement well. The number of paths was increased until all the peaks were matched. Although providing a good starting point, that analysis has limited physical significance because no simultaneous analysis of the paths was attempted. The tracer data alone were not sufficient for Benson [1988] to determine the three-dimensional structure of conductivity at this site. Our method indicates that the full three-dimensional flow and transport system can be described using the cross-well seismic data to help parameterize the hydrogeologic inversion. Tracer simulations using the estimates of the heterogeneous conductivity field provide a significantly better fit to the tracer concentration histories than homogeneous estimates. It may be possible to develop finely layered conductivity estimates that provide a good fit to the tracer data; however, this would be inconsistent with the significant lateral heterogeneity observed by Benson et al. [1991]. Lateral conductivity variations were also observed as differences between two perpendicular tracer tests at the study site [Benson, 1988]. Benson [1988] estimated the longitudinal dispersivities to be on the order of 3 cm for this site, which is somewhat less than our estimate of 9 cm determined from sensitivity analysis.

### Sensitivity Analysis

We estimated the longitudinal dispersivity using sensitivity analysis, rather than including this as a parameter in the inversion, to substantially reduce the computation. For a particular dispersivity value the objective function (4) was minimized by adjusting the slowness values that determine the zonation of the aquifer, called seismic slowness splits, and the zonal conductivity values. With this approach we used longitudinal dispersivity values in the range of 0.5 to 30 cm and found that a value near 9 cm best matched the observed data. Changing the dispersivity had little effect on the optimal hydraulic conductivity and slowness split values chosen but did change the shape of the concentration arrival histories. If the peaks are too

**Figure 4.** Distribution of hydraulic conductivity estimates obtained from the split inversion method. For this realization the estimated slowness splits are 569.4 and 587.8 μs/m, and the hydraulic conductivity values are $1.4 \times 10^{-4}$ m/s for the dark gray regions, $3.6 \times 10^{-4}$ m/s for the gray regions, and $5.0 \times 10^{-4}$ m/s for the light gray regions. For reference, the seismic cross sections are below the white lines and the vertical line denotes the location of well 4.
broad and the peak magnitudes are lower than those observed, the dispersivity estimate is too large and thus should be reduced. The transverse dispersivity value was fixed at 0.2 times the longitudinal value, which achieved slightly better fits to the concentration histories than simulations that used 0.1 times the longitudinal value.

To illustrate the sensitivity of the objective function to the zonation of aquifer properties, the two slowness splits are adjusted with all other parameters held constant. Figure 6 demonstrates how tracer concentration residuals change non-linearly owing to changes in the slowness splits, which determine the zonation for hydraulic conductivity. Although several local minima are apparent in these sensitivity plots, the SIM appears to have converged to a global minimum with respect to these parameters.

The optimum parameter set for the Kesterson inversion (Table 2) appears to provide a global minimum of the specified objective function (4) with respect to the zonal conductivity values. The tracer data provided sensitivity to the conductivity differences between zones and the geometry of these zones, while the drawdown data provided sensitivity to the average value of hydraulic conductivity at the site.

This emphasizes the need to collect hydraulic head data during tracer tests, such as the measured drawdown of 0.15 m at well HO60 during the 1986 tracer test. In cases with no constraint on the hydraulic gradients, reducing the average conductivity while using constant head boundaries increases proportionally the hydraulic gradient in order to achieve the same total flow rate. This results in approximately the same average fluid and tracer velocities. At the Kesterson site this single measured drawdown value constrained the hydraulic gradients at the site, which allowed us to estimate the average conductivity as well as the differences between zones. Additional drawdown measurements would have been useful to further refine our conductivity estimates at the site.

We also examined the sensitivity of the tracer concentrations to the horizontal and vertical correlation lengths as well as the type of variogram used (exponential and Gaussian). We tried horizontal correlation lengths of 1, 5, 9, and 18 m, with vertical correlation lengths of either 0.1, 0.5, or 0.9 m. None of these sets of geostatistical parameters reproduced the tracer concentration histories as well as the realizations generated with an exponential variogram with \( \lambda_x = 9 \) m, \( \lambda_z = 0.9 \) m, and \( \sigma^2 = 104 \). The correlation lengths estimated from the seismic tomosgrams thus appeared to provide information about the correlation of hydraulic properties. Clearly, more long tomograms would have facilitated the estimation of horizontal correlation lengths. Although the relation between seismic and hydraulic parameters is unknown, the size and shape of the lithologic zones appear to be imaged with seismic data. Different lithologies are likely to have different hydraulic properties, and thus the seismic information is likely to provide information about the spatial correlation of the hydraulic conductivity field. The cross-well seismic estimates also provided a reasonable initial estimate of the horizontal correlation length.

Summary and Conclusions

We have demonstrated the split inversion method (SIM) to combine seismic, hydraulic, and tracer data to estimate the lithologic zonation of the Kesterson aquifer, estimate the hydraulic conductivity for each zone, and estimate the dispersivity for the region. This is the first paper that we know of that combines seismic, hydraulic, and tracer data to estimate the three-dimensional hydraulic conductivity structure of an aquifer. The SIM adjusts five parameters to obtain the best fit to tracer concentration histories. These parameters are two values that split seismic slowness realizations into three populations and three hydraulic conductivity values, one for each population. Other parameters are determined using sensitivity analysis, such as the regional value of dispersivity and the horizontal and vertical correlation lengths at the site.

The results demonstrate that combining seismic and tracer data has the potential to provide high-resolution estimates of aquifer zonation and hydraulic properties for some aquifers. The seismic data provide three-dimensional estimates of the aquifer structure even though the relationship between seismic slowness and the hydraulic parameters of interest is unknown. The tracer data allow us to split the slowness estimates into a small number (determined from prior information) of geologically reasonable zones in three dimensions and assign flow and transport properties to the zones. By combining seismic and tracer data, we were able to obtain more information about subsurface properties than if we had used either data set alone.

Several objective functions were attempted for this Kesterson inversion to provide rapid convergence. The best conver-
gence was obtained by minimizing the squared difference between arrival time quantiles from the concentration histories. This objective converges even if the starting estimates are far from optimal. The minimum absolute value of concentration residuals was originally used for the objective function, but this objective did not converge. We then minimized the squared concentration residuals, which converged if the starting estimates were fairly close to the optimal values. This least squares approach had problems with local minima because the objective heavily penalized simulated peaks of the proper magnitude, even if they were slightly offset from the measured peaks. The highest peaks also dominated the solution; thus the parameter estimates from this objective may not provide an optimal solution for all the measured concentration histories. It is important to examine the fit to the data for a variety of parameter sets to help develop the best objective function. Some objective functions will not converge toward accurate fits to the data, and overly complicated objectives may have competing factors that hamper convergence. The objective could include many other indices of the concentration arrival histories, such as peak concentration arrival times as presented by Hyndman et al. [1994], peak magnitudes, and temporal moments of the concentration histories.

As discussed in the results section, tracer concentration histories between an injection/withdrawal well pair provide information that can be used to determine the relative hydraulic conductivities for a site. However, these data are fairly insensitive to the magnitude of the mean hydraulic conductivity if the boundary conditions are also unknown. There are several ways around this problem, including (1) collecting multiple sources of data, such as tracer concentrations and hydraulic

Figure 6. Sensitivity of the objective value (squared concentration residuals) to the two values of seismic slowness split that determine the zonation of hydraulic conductivity along a west-to-east cross section through the three dimensional estimate. (a) Sensitivity to the low slowness split (between gray and dark gray on Figure 4). (b) Sensitivity to the high slowness split (between gray and light gray on Figure 4).
head measurements; (2) determining values of specified flux boundaries for the site; and (3) using pumping test data to constrain the mean conductivity values. Detailed hydraulic head measurements, which are easy to collect and do not require expensive analyses, constrain the average hydraulic conductivity. Hydraulic head data could also be used to constrain the potential range of hydraulic conductivity values before using the much more numerically expensive tracer simulations.

Although the SIM was presented for seismic travel times, tracer concentrations, and drawdown, many other applications are possible. Other hydrologic data, such as transient hydraulic head measurements, could be used instead of (or in addition to) tracer concentrations. Other seismic attributes can also be inverted to obtain more information about hydraulic properties. For example, measured seismic amplitudes and frequencies can be used to estimate attenuation coefficients. These coefficients are likely correlated to hydraulic conductivity because the ease of fluid movement affects the attenuation of seismic energy. Geophysical methods, such as ground-penetrating radar and cross-well resistivity, should also provide valuable data sets to help delineate aquifer structure and properties for different geological regimes. Ground-penetrating radar works best when the clay content of the soil is low, although cross-well radar methods may allow us to image the structure of sand zones between clay lenses with very high resolution.

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