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Journal of Contaminant Hydrology 85 (2006) 72 – 88

JOURNAL OF
Contaminant
Hydrology

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Geophysical constraints on contaminant transport modeling in a heterogeneous fluvial aquifer

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Received 1 November 2004; received in revised form 14 January 2006; accepted 20 January 2006

Abstract

Approximately 3000 measurements of hydraulic conductivity in over 50 flowmeter boreholes were available at the Macro-Dispersion Experiment (MADE) site in Columbus, Mississippi, USA to quantify the heterogeneity in hydraulic conductivity at the site scale. This high-density measurement approach is perhaps infeasible for time and expense in typical groundwater remediation sites. A natural-gradient tracer experiment from the MADE site was simulated by a groundwater flow and solute transport model incorporating direct-current (DC) resistivity data collected over the observed plume location. Hydraulic conductivity from one borehole collected during the original site characterization was used to calibrate the electrical resistivity data to hydraulic conductivity using a previously derived log–log relationship. Application of this relationship, using site-specific empirical constants determined from the data, transforms the 3D electrical resistivity data into a 3D description of hydraulic conductivity that can be used in groundwater models. The validity of this approach was tested by using the geophysically derived hydraulic conductivity representation in numerical simulations of the natural-gradient tracer experiment. The agreement between the simulated and observed tracer plumes was quantified to gauge the effectiveness of geophysically derived and flowmeter based representations of the hydraulic conductivity field. This study demonstrates that a highly heterogeneous aquifer can be modeled with minimal hydrological data supplemented with geophysical data at least as well as previous models of the site using purely hydrologic data.

Keywords: Hydrogeophysics; Resistivity; Contaminant transport modeling; Aquifer heterogeneity; MADE site

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doi:10.1016/j.jconhyd.2006.01.006

1. Introduction

Large-scale tracer tests in natural systems have been conducted in a variety of depositional environments. These tracer tests are generally constrained by extensive subsurface hydrologic data (e.g., borehole flowmeter measurements, pump tests, grain-size analysis, etc.), and are designed as case studies to characterize aquifer flow and transport properties and processes so that they can guide groundwater management at other similar sites where much less subsurface information is available.

Tracer tests, such as the one examined in this paper, are indispensable in hydrogeologic investigations, but they require detailed site characterization and collection of a large amount of hydraulic conductivity data. This is particularly true in heterogeneous environments, where hydraulic conductivity variations may be extreme over distances that are short compared to the transport path. Collecting such data with conventional hydrogeologic methods (e.g., boreholes) can be very costly.

Surface geophysical methods (e.g., electrical, radar, and seismic methods) provide an alternative to expensive borehole data to obtain dense spatial coverage, albeit with only indirect links to subsurface hydrological attributes such as hydraulic conductivity, porosity, and pore fluid composition. Qualitative, and occasionally quantitative, relationships can often be found between geophysical and hydrological attributes, particularly in regards to estimating lithology and hydraulic conductivity from resistivity data (e.g., Heigold et al., 1979; Kosinski and Kelly, 1981; Urish, 1981; Ponzini et al., 1983; Frohlich et al., 1996). In many cases, a simple log–log relationship can be established between electrical (c) and hydraulic (K) conductivities (Purvance and Andricevic, 2000). When such a relationship can be established, geophysical studies can be used to provide an inexpensive subsurface hydraulic conductivity image that can be used as an input parameter to groundwater flow and contaminant transport models.

This paper examines the use of areally extensive geophysical measurements made with direct-current (DC) resistivity at the Macro-Dispersion Experiment (MADE) site in Columbus, Mississippi, USA and their application to constraining contaminant transport models of a natural gradient tritium tracer test. The objective is to establish the extent to which surface geophysical data, correlated with limited hydrologic borehole data, can be used as a proxy for dense borehole measurements in groundwater flow and transport modeling in heterogeneous aquifer systems. Transport simulations based on two modeling approaches, the advection–dispersion model (ADM) and the dual-domain mass transfer model (DDMT), are used to compare three methods of representing the hydraulic conductivity field. The agreement between the simulated plume and the observed MADE-2 tritium plume is quantified to gauge the effectiveness of each representation of the K field.

The first method of representation (K1) treats the K field as a layered distribution in which the hydraulic conductivity of each layer in the numerical model is constant, and is determined from the average K values taken from a single borehole flowmeter log without using any geophysical constraints. The second method of representation (K2) builds upon the first method (K1) by augmenting the description of the hydraulic conductivity field over a portion of the MADE site covered by a surface resistivity survey. Hydraulic conductivity within this area of K2 is determined from an empirical relationship between DC resistivity and hydraulic conductivity that was calibrated to the K values from the same borehole flowmeter log as K1. The hydraulic conductivity values vary in three dimensions inside the geophysical survey area but outside of the geophysical survey area they are constant in each model layer and remain the same as in K1. The third method of representation (K3) is similar to previous modeling of the MADE site (Feehley et al., 2000) that uses kriging interpolation and the abundant hydraulic conductivity measurements to develop a three-dimensional K distribution based on purely hydrologic data.

2. Description of the site and tracer test

2.1. Site description

The MADE site is located on terraced fluvial deposits (Cook, 1998) between the Tombigbee and Buttahatchee Rivers in the northeastern part of Mississippi (see the inset in Fig. 1). The aquifer consists of all sediments above the clay member in the lower bounding Eutaw Formation that acts as an aquitard (Boggs et al., 1990; Boggs and Adams, 1992). The depth to the base of the aquifer averages 11 m but varies between 10 and 16 m (Boggs et al., 1990).

Recent geophysical studies based on direct-current (DC) resistivity as well as ground penetrating radar (GPR) at a nearby active sand and gravel quarry and the MADE site itself have produced a detailed depositional and hydrogeological model of the aquifer (Bowling, 2005; Bowling et al., 2005). Based on the resistivity data (see Figs. 1 and 2) and additional information obtained in those studies, Bowling et al. (2005) divided the MADE site into four stratigraphic units: 1) an upper layer of meandering fluvial sediments (MFS) showing a recently dug trench and a relict channel with clay fill, 2) an upper-middle layer of high resistivity associated with gravelly sands deposited by a braided fluvial system (BFS), 3) a moderate resistivity layer associated with fine sands and silts of the Eutaw Formation (Eutaw Sand), and 4) a low resistivity layer associated with the high clay content of the Eutaw Formation (Eutaw Clay).

The top two units were deposited by a meandering fluvial system (MFS) and braided fluvial system (BFS), respectively, while the lower two units are part of the Eutaw Formation (Fig. 2). According to Bowling et al. (2005), radar stratigraphy of the second unit consists of multiple lenticular bodies, bound by radar surfaces of various scales and continuity. The lenticular bodies are on the order of 5–10 m in length and typify deposits by a braided fluvial system. This unit is the main aquifer at the MADE site and accounts for the considerable heterogeneities in hydraulic conductivity that have been reported (Rehfeldt et al., 1992).

2.2. Tracer test

There have been three large-scale natural-gradient tracer experiments performed at the MADE site; two macro-dispersion experiments (MADE-1 and MADE-2; October 1986 through June 1988 and June 1990 to September 1991, respectively) and a natural attenuation study (NATS; August 1995 to September 1997) (e.g., Boggs et al., 1990; Boggs and Adams, 1992; Boggs et al., 1993; MacIntyre et al., 1993; Feehley et al., 2000; Julian et al., 2001). One of the major goals of these studies was to test fluid-flow and transport models against flow and transport data collected in a densely instrumented monitoring network.

This study uses tracer concentration data from the second experiment (MADE-2) as a benchmark to compare results of groundwater flow and contaminant transport models that are based on different hydraulic conductivity representations derived from the geophysical data. During the MADE-2 experiment, a tracer solution with a tritium concentration of 55,610 pCi mL^{-1} was injected into the aquifer at a constant rate of 3.3 L min^{-1} for 48.5 h at a depth of 7.4–8.0 m. The total tritium mass injected by five wells spaced 1 m apart was 0.5387 Ci (Boggs et al., 1993). Monitoring the evolution of tritium concentrations in the

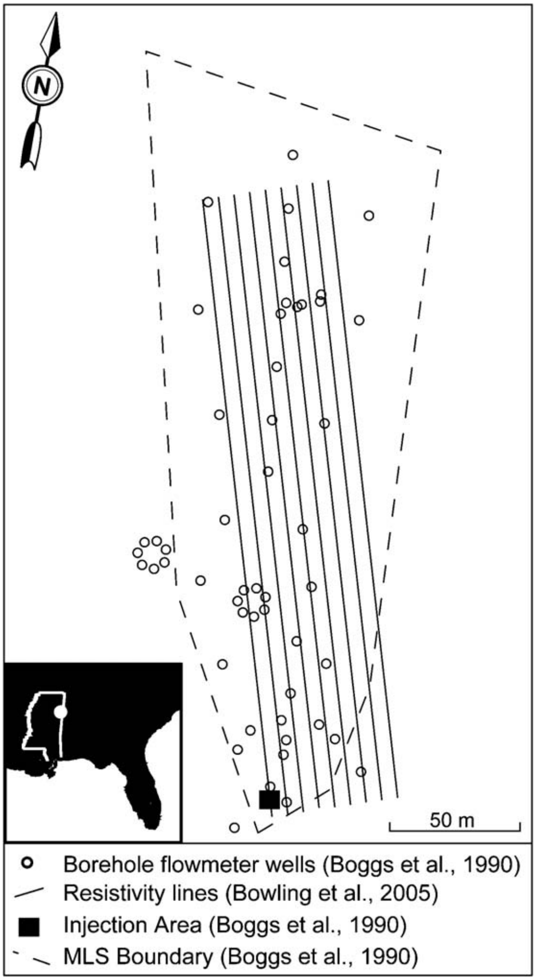


Fig. 1. Direct current resistivity surveys collected at the MADE site in Columbus Air Force Base in Mississippi. Dense vegetation inhibited data collection in the western, northern, and northeastern portions of the site. Also shown for reference are the site boundary (dashed line) and locations of flowmeter wells where hydraulic conductivity measurements (open circles) were taken (Boggs et al., 1990).

aquifer was accomplished by a network of multilevel samplers that sampled the groundwater at over 300 surface locations and over 6000 vertical points. Comparison of model predictions to tritium concentrations observed 328 days after source injection is used to judge the effectiveness of the flow and transport models.

2.3. Observed tritium plume

Observations of tritium concentrations show a distinctive non-Gaussian longitudinal distribution (Fig. 3) that is attributed to the aquifer's extreme heterogeneity (e.g., Feehley et al., 2000). Even after 328 days, a majority of the tracer remained within 6 m of the injection point with a diffuse, low concentration zone extending for more than 200 m down gradient. Two factors

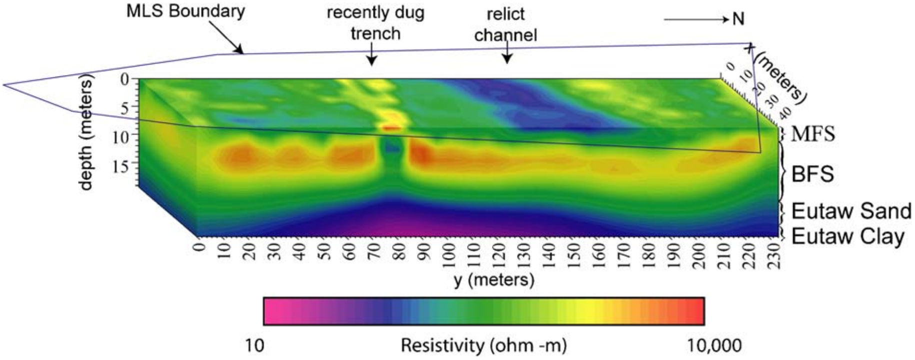


Fig. 2. Three-dimensional DC resistivity image of the MADE site (after Bowling et al., 2005). Based on the resistivity data and additional information not shown, the MADE site can be divided into four main facies: 1) meandering fluvial sediments (MFS), 2) braided fluvial system (BFS), 3) Eutaw Silt and Sand, and 4) Eutaw Clay.

may have contributed to these characteristics. First, the injection wells were located in a zone of relatively low hydraulic conductivity, which restricted movement of the bulk of the tracer (Boggs et al., 1993). Second, preferential flow pathways believed to exist among high-K sediments in the aquifer resulted in diffuse spreading of low-concentrations of tritium down gradient (e.g., Feehley et al., 2000; Harvey and Gorelick, 2000; Zheng and Gorelick, 2003).

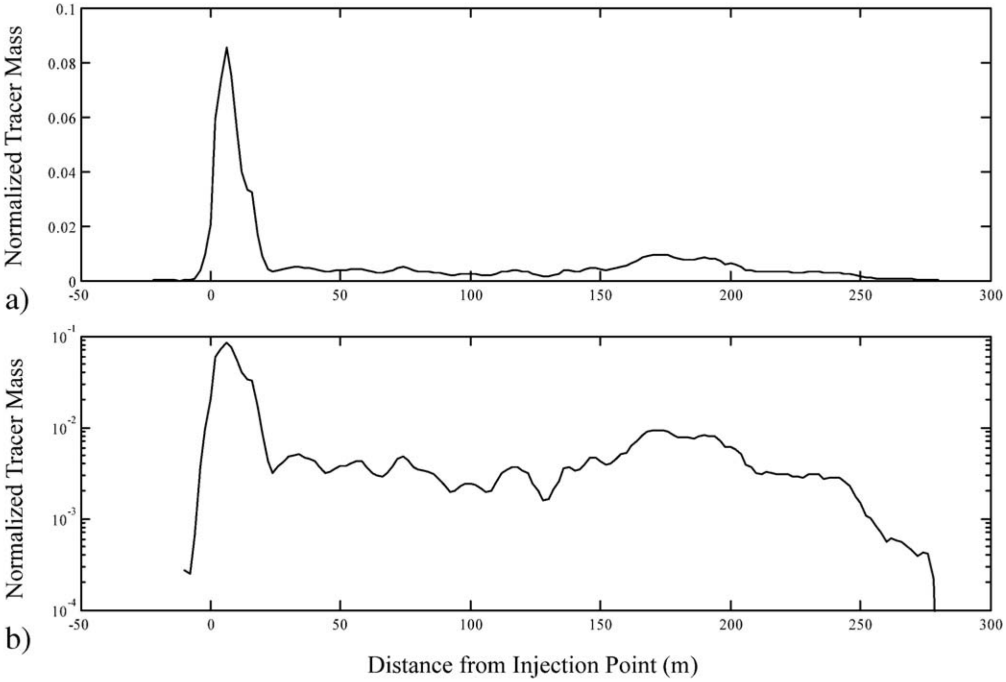


Fig. 3. A one-dimensional laterally and vertically integrated mass profile along the general groundwater flow direction, based on observed tritium concentrations during the second MADE experiment at 328 days after initial injection of the tracer. The normalized tracer mass is shown in both a) normal and b) logarithmic scales to highlight low concentrations of the tritium plume down gradient of the injection point.

3. Hydrological and geophysical data

3.1. Hydrological data

More than 3000 measurements of hydraulic conductivity have been made at the MADE site using borehole flowmeters (Boggs et al., 1990; Rehfeldt et al., 1992). Generally, hydraulic conductivity measurements were taken every 15 cm vertically between the water table and clay aquitard of the Eutaw Formation. Hydraulic conductivity typically ranges 3 to 4 orders of magnitude in a single well (Rehfeldt et al., 1992) as illustrated by well K-39 (Fig. 4). A layer-averaged representation in which a uniform hydraulic conductivity value for each layer of the

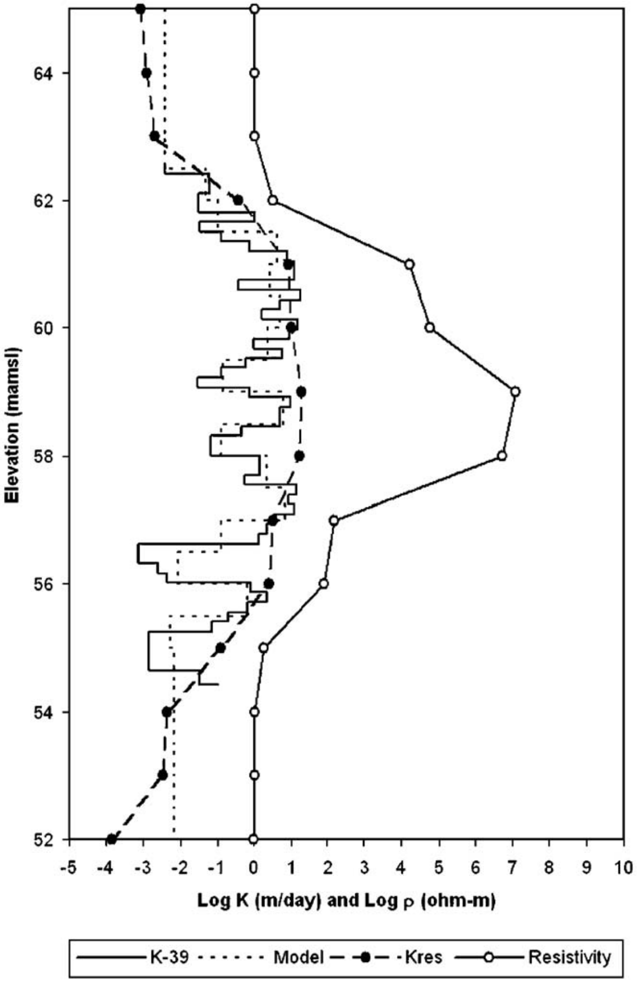


Fig. 4. Distribution of measured hydraulic conductivity values (solid line) in a single flowmeter well (K-39). The dashed line shows the averaged hydraulic conductivity values over 0.5 m increments to provide input to the homogeneous layered models. A resistivity trace from the inverted data volume near the location of K-39 shows a similar trend with depth (the solid line connected by open circles represents the raw resistivity data in ohm-m while the dashed line connected by solid dots represents the scaled resistivity data correlated to the flowmeter hydraulic conductivity distribution).

groundwater flow and contaminant transport models is derived from this well serves as a baseline for comparison with other more complex representations examined in this work.

3.2. Geophysical data

The geophysical data set used in this study consists of nine 2D DC resistivity lines (Fig. 1). Resistivity data were collected with an electrode spacing of 5 m in a dipole–dipole configuration with individual survey lines spaced 6 m apart. All nine resistivity lines were simultaneously inverted to produce a pseudo 3D data volume (Fig. 2). The inversion was done on a model grid of 1.75 m vertical by 5 m horizontal using the Geotom software RES3DINV (http://www.geoelectrical.com). Detailed information regarding processing, inversion, and lithostratigraphic interpretation of the geophysical data can be found in Bowling et al. (2005). Bowling et al. (2005) also noted a qualitative relationship between resistivity and hydraulic conductivity, with depth-averaged resistivity profiles exhibiting similar trends as the depth-averaged hydraulic conductivity data. This association suggests a possible quantitative relationship between hydraulic conductivity and DC resistivity, which is exploited in the groundwater flow and contaminant transport models.

3.3. Geophysical–hydrological relationships

Extensive research has been conducted in search of a quantitative relationship between electrical resistivity and hydraulic conductivity (e.g., Kelly, 1977; Heigold et al., 1979; Kelly and Frohlich, 1985; Ahmed et al., 1988; Cassiani and Medina, 1997; Purvance and Andricevic, 2000; Yeh et al., 2002; Niwas and de Lima, 2003). Purvance and Andricevic (2000) described a log–log relationship based on Archie's law and the Kozeny–Carmen equation (Scheidegger, 1974) of the form

$$\log(K) = \frac{\log(\mathrm{Res})}{A} + B \tag{1}$$

where A and B are statistically or experimentally determined constants. A and B were determined by forward modeling, using resistivity values extracted from the inverted resistivity volume and hydraulic conductivity data from well K-39. Values of 0.3 and -10.0 for A and B, respectively, produce a satisfactory match to the hydraulic conductivity data of well K-39 (Fig. 4). The log–log relationship based on well K-39 was used to convert the three-dimensional electrical resistivity image into a three-dimensional hydraulic conductivity field. The hydraulic conductivity profile estimated from the resistivity data (K_{res}) agrees with the observed hydraulic conductivity profile at well K-39 to a first order, but does not resolve higher order fluctuations. However, these fluctuations occur over vertical intervals of less than 0.5 m, the smallest vertical discretization that can be explicitly represented in the flow and transport models developed for the MADE site (Feehley et al., 2000).

4. Modeling method

4.1. Conceptual models

The MADE-2 experiment (Boggs et al., 1993; MacIntyre et al., 1993) was simulated with two modeling approaches, the advection–dispersion model (ADM) and the dual-domain mass transfer model (DDMT). The advection–dispersion model assumes that the average velocity of the tracer equals the average velocity of groundwater, but allows for small deviations from the average velocity caused by local heterogeneities that are below the grid spacing of the model. The advection–dispersion model assumes all pore water is mobile and uses only a single porosity to characterize the transport regime. The single-porosity advection–dispersion model has been applied to the MADE site by Zheng and Jiao (1998), Eggleston and Rojstaczer (1998), and Barlebo et al. (2004). Zheng and Jiao (1998) noted that the ADM can reproduce reasonably well the observed MADE-2 tritium plume above a certain concentration limit, but it fails to reproduce the extensive downstream spreading of the tracer plume at low concentrations. Eggleston and Rojstaczer (1998) also pointed out this limitation of the ADM. Barlebo et al. (2004) showed that the agreement between the ADM and the observed plume can be improved somewhat if the K distribution is obtained through model calibration rather than directly from the flowmeter measurements. The application of the ADM in this study is intended to investigate whether or not the use of geophysical data, with a better spatial coverage than hydrologic data, can improve the effectiveness of the ADM in reproducing the observed MADE-2 tritium plume while honoring the flowmeter K measurements.

The DDMT model has been shown to be able to reproduce the observed extensive downstream spreading of the tracer at low concentrations while retaining high concentrations near the injection point (e.g., Harvey, 1996; Harvey and Gorelick, 2000; Feehley et al., 2000). The DDMT model overcomes the inability of the advection–dispersion model to account for preferential flow paths operating below the grid spacing of the numerical model by partitioning the aquifer medium into mobile and immobile fluid domains. The mass exchange between the two domains is governed by a first-order mass transfer equation with a given rate coefficient (β) (Griffioen et al., 1998). To fully test the applicability of geophysical data as constraints on groundwater models, both ADM and DDMT models are used here to simulate contaminant transport based on the MT3DMS code (Zheng and Wang, 1999).

4.2. Spatial discretization

A three-dimensional block-centered finite difference grid was used for modeling the site. A model domain from the coordinate −72.5 to 32.5 m in the east–west direction and −37.5 to 292.5 m in the north–south direction was chosen for consistency with prior modeling studies of the MADE-2 experiment. The origin is located at the injection area (Fig. 5). The model domain was divided horizontally into 68 columns and 152 rows with variable grid spacing. Interior grid cells were 2 m × 2 m with grid dimensions progressively increased to 3, 4.5, 6, and 9 m toward both edges of the model domain. The top of the model was topographically flat with an elevation of 65 m above mean sea level. The bottom of the model was at the interface between the shallow fluvial deposits and the Eutaw clay formation which was approximately treated as a flat plane at 48 m above mean sea level. The model was discretized into 34 layers, with a vertical grid spacing of 0.5 m. The maximum model depth of 17 m was chosen based on hydrogeologic and geophysical information.

4.3. Boundary and initial conditions

Boundary conditions for the steady-state flow model consist of specified-head boundaries to the north and south and no-flow boundaries to the east and west (Fig. 5). Specified heads at the northern and southern boundaries were interpolated from average heads of 1-year observations at 48 piezometers installed at the MADE site using ordinary kriging. A no-flow boundary is also

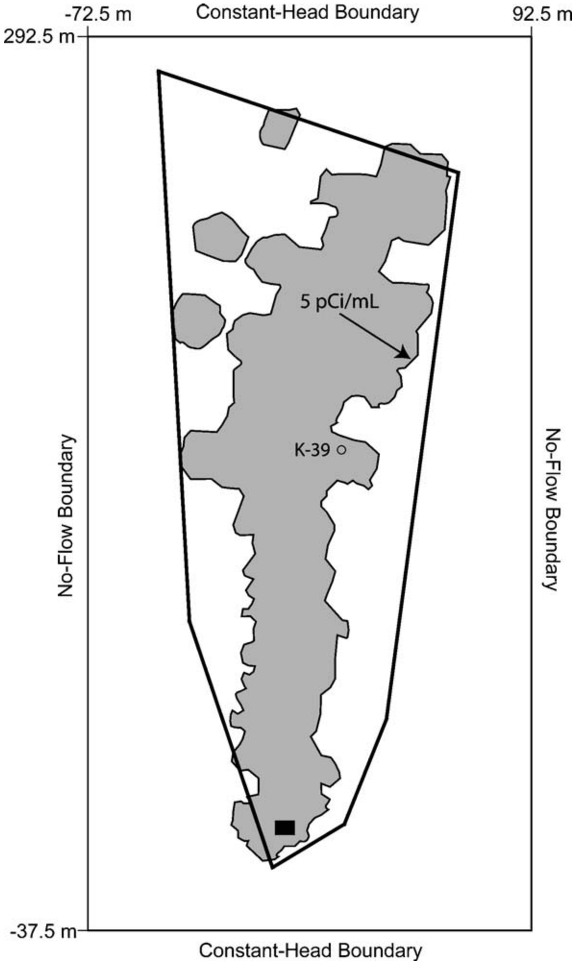


Fig. 5. The finite difference model grid used to simulate the MADE-2 tritium tracer experiment. Also shown are the tracer injection point and the 5-pCi/mL outer limit of the tritium plume at any depth 328 days after the initial injection. Flow boundary conditions are specified-head to the north and south and no-flow to the east and west. Transport boundary conditions are zero-mass-flux on all boundaries except to the north where the advective mass flux is specified.

specified at the base of the model between the shallow fluvial aquifer and the aquitard of the Eutaw formation, and a specified recharge flux is imposed at the top of the model. Boundary conditions for the transport model are zero-mass-flux on all boundaries except for the northern boundary where the solute can exit freely out of the model domain.

4.4. Transport parameters

For the advection–dispersion models, the longitudinal dispersivity was assigned a value of either 1 or 5 m. Ratios of horizontal transverse and vertical dispersivities to the longitudinal dispersivity were set equal to 0.01 and 0.001, respectively. These values were based on Zheng and Jiao (1998) and Feehley et al. (2000). For the dual-domain model, the longitudinal dispersivity was set at the lower value of 1 m. The ratios of horizontal transverse and vertical dispersivities to the longitudinal dispersivity were the same as in the advection–dispersion models. Mass transfer rate coefficients of 0.001 and 0.0005 day^{-1} have been shown to be applicable to the MADE site (Feehley et al., 2000; Julian et al., 2001), and were used in this study. A lower mass transfer rate coefficient of 0.0001 day^{-1} was also examined. In addition, the ratio of mobile to total porosities was set at 1 to 8 based on the previous work of Feehley et al. (2000).

4.5. Simulation procedure

Both advection–dispersion simulations and dual-domain simulations of the tritium plume were used to test various representations of the hydraulic conductivity field. A total of 15 simulations were conducted by combining model-type, dispersivity, and mass-transfer rate coefficient (β) (Table 1).

As described previously, three representations of the hydraulic conductivity field were used to test the ability of the advection–dispersion and dual-domain mass transfer models to adequately simulate the tracer experiment using minimal borehole data. The first representation (K1) is a laterally homogeneous distribution that uses one single average hydraulic conductivity value determined from well K-39 to define each of the vertical layers (see Fig. 4). The second representation (K2) builds upon the first representation by incorporating a heterogeneous K field derived from the resistivity data (K_{res}) over the region where resistivity data were collected (Fig. 2). Outside the resistivity survey area, the hydraulic conductivity was defined as in K1. This was necessary because dense foliage and man-made structures (e.g., buildings, roads, etc.) prevented collection of resistivity data in all portions of the test site. A third representation (K3) of the hydraulic conductivity field is based entirely on ordinary kriging interpolation of hydraulic conductivity data from over 50 flowmeter wells at the MADE site. This representation is similar to that used in other studies (e.g., Feehley et al., 2000), and allows for comparison of transport models based on geophysically derived hydraulic conductivity representation (K2) with those based on direct hydrologic flowmeter measurements (K3).

Table 1
Input parameters and output statistics for various simulation scenarios

Model	Type[a]	Dispersivity[b] (m)	β (day^{-1})	r	Mass remaining[c]
K1a	AD	1, 0.01, 0.001	n/a	0.24	1.00
K1b	AD	5, 0.05, 0.005	n/a	0.18	0.99
K1c	DD	1, 0.01, 0.001	0.0010	0.43	1.00
K1d	DD	1, 0.01, 0.001	0.0005	0.52	1.00
K1e	DD	1, 0.01, 0.001	0.0001	0.60	0.99
K2a	AD	1, 0.01, 0.001	n/a	0.39	1.00
K2b	AD	5, 0.05,0.005	n/a	0.38	1.00
K2c	DD	1, 0.01, 0.001	0.0010	0.63	0.96
K2d	DD	1, 0.01, 0.001	0.0005	0.64	0.88
K2e	DD	1, 0.01, 0.001	0.0001	0.63	0.57
K3a	AD	1, 0.01, 0.001	n/a	0.31	1.00
K3b	AD	5, 0.05, 0.005	n/a	0.20	1.00
K3c	DD	1, 0.01, 0.001	0.0010	0.62	1.01
K3d	DD	1, 0.01, 0.001	0.0005	0.62	0.99
K3e	DD	1, 0.01, 0.001	0.0001	0.59	0.87

[a] AD = Advection–dispersion model, DD = Dual-domain mass transfer model.

[b] Values represent (longitudinal, horizontal transverse, and vertical) dispersivities.

[c] Mass remaining calculated as the total calculated mass remaining in the aquifer at 328 days normalized by the total initially injected mass.

4.6. Mass distribution

The mass injected in the simulations was the same as that used in the original experiment. For easier comparison of the simulated plumes with the observed tritium plume, an integrated 1D mass profile is created by integrating the calculated tritium mass distribution in the transverse

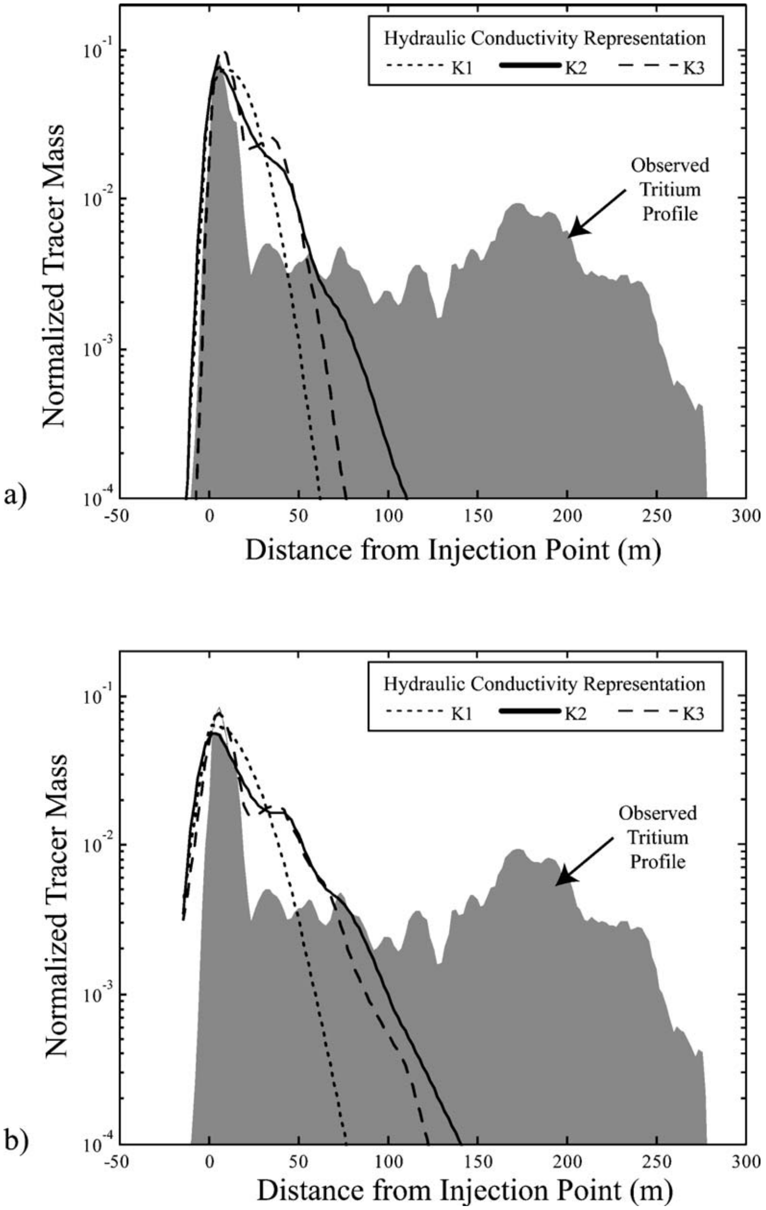


Fig. 6. Results of simulations using the advection–dispersion transport model and each of the three *K* representations grouped by simulations with a longitudinal dispersivity of a) 1 m and b) 5 m. Model parameters are given in Table 1.

direction (perpendicular to the flow direction) and the vertical direction along a profile trending down gradient and passing through the injection point. The 1D mass profile 328 days after the tracer was injected is then normalized by the total mass injected such that the area under each model curve is equal to 1. This normalized mass profile is compared to a similarly constructed profile calculated from the observed tritium plume. For the dual-domain model, the simulated 1D mass profile includes mass in both the mobile and immobile domains. The MADE site tracer tests

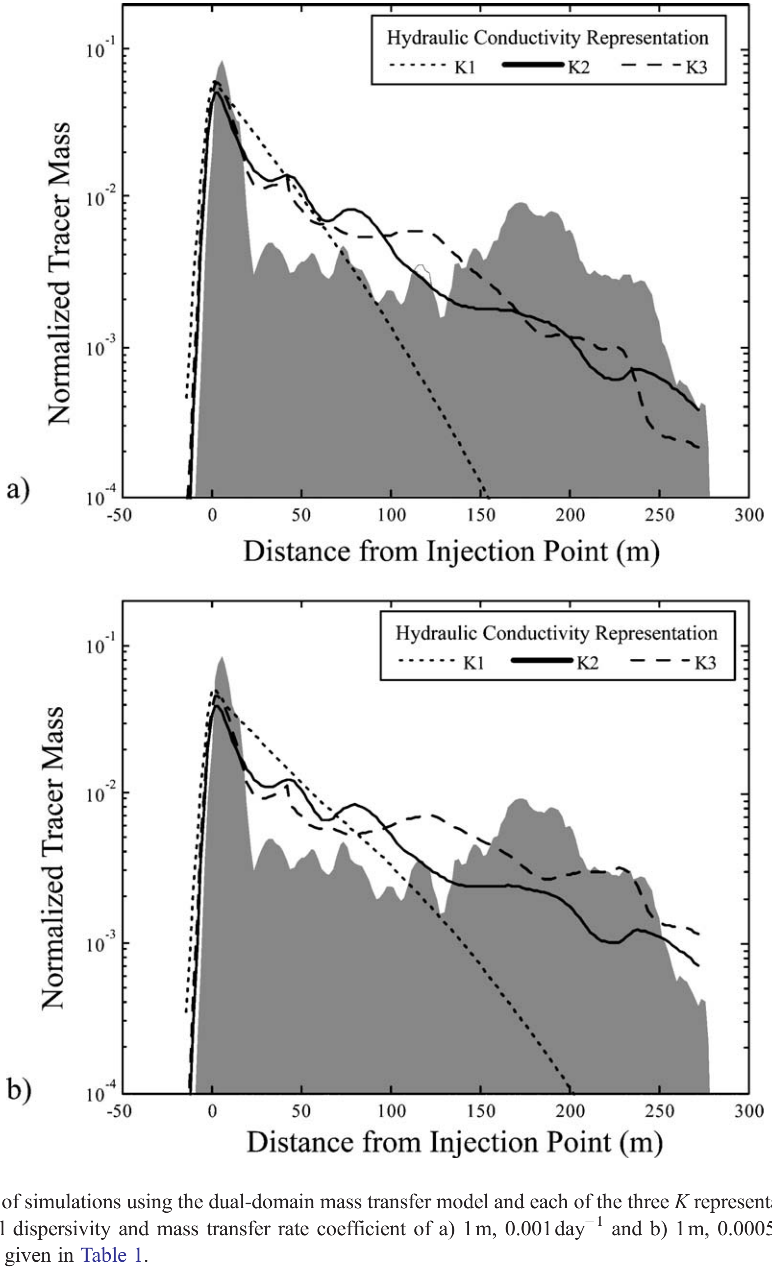


Fig. 7. Results of simulations using the dual-domain mass transfer model and each of the three K representations grouped by longitudinal dispersivity and mass transfer rate coefficient of a) 1 m, 0.001 day^{-1} and b) 1 m, 0.0005 day^{-1}. Model parameters are given in Table 1.

were monitored over time to ensure that substantial tracer had not left the observation network. As such, the mass of tracer injected and the mass predicted in the aquifer at the end of the simulation period (328 days) are compared to verify that no significant amount of tritium mass has left the model domain.

5. Results and discussion

5.1. Assessing goodness of the model fit

The simulation results are qualitatively compared based on the amplitude and location of the peak in the 1D mass profiles and the presence and characteristic of the low-concentration spreading down gradient of the peak in the mass profiles. The correlation coefficient (r) between the observed and calculated mass distributions is computed and used as the quantitative measure of the agreement between the two distributions:

$$r = \frac{\sum_{k=1}^{N} \left(\log M_{1,k} - \overline{\log M_1}\right)\left(\log M_{2,k} - \overline{\log M_2}\right)}{\sqrt{\sum_{k=1}^{N} \left(\log M_{1,k} - \overline{\log M_1}\right)^2} \sqrt{\sum_{k=1}^{N} \left(\log M_{2,k} - \overline{\log M_2}\right)^2}} \tag{2}$$

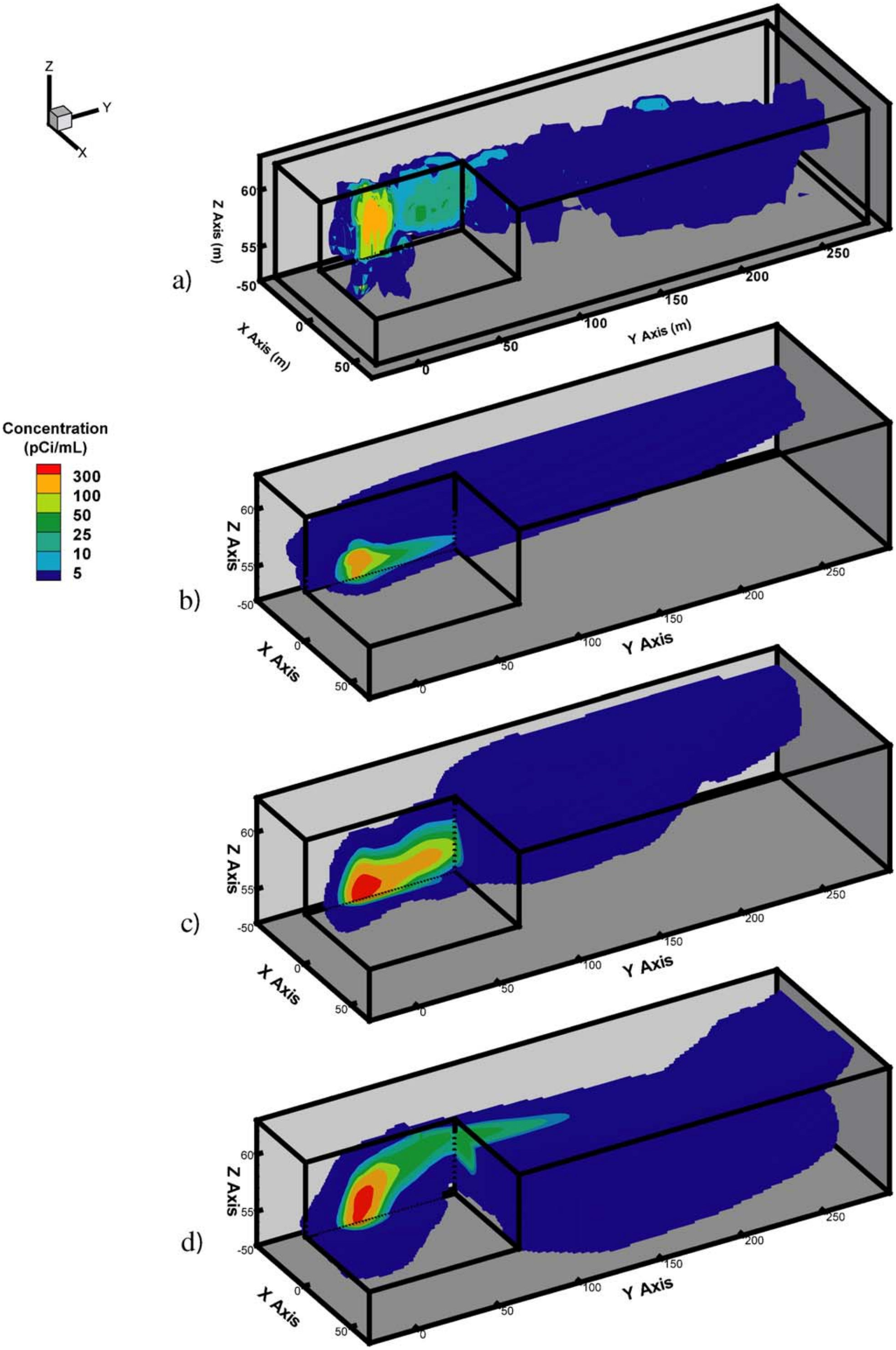
where M_1 and M_2 refer to the observed and calculated mass, respectively. For the dual-domain models, M_2 represents the sum of the mass in both mobile and immobile domains. Use of the logarithm of the mass prevents the correlation coefficient from being dominated by a few high peak values. An r value of 1 indicates a perfect match while a value of 0 indicates no match at all.

The correlation coefficients for the observed and calculated tritium plumes range from 0.18 to 0.64 (Figs. 6 and 7; Table 1). In general, the dual-domain model results in significantly higher r values than the advection–dispersion models.

5.2. Advection–dispersion simulations

Advection–dispersion simulations based on the three K representations all produce a reasonably good agreement between the observed and calculated peak concentrations but fail to reproduce the low concentrations of tritium observed at distances much greater than 100 m from the injection point (Fig. 6). Quantitative comparison of six simulations to the observed tritium profile have an r value ranging from 0.18 to 0.39 (Table 1). Simulations with the layered uniform K distribution (K1 conductivity representation) show a monotonic decrease in plume mass downgradient and lack the roughness (non-monotonic variations in plume mass) observed in the data. However, simulations with the geophysically based and flowmeter based K distributions (K2 and K3) have more variation to their profiles. The skewness in the mass profile (displacement of mass downstream relative to the peak mass) is greatest in the model using the K2 conductivity representation.

Fig. 8. Comparison of observed and calculated tritium plumes at 328 days: a) observed; b) based on K1; c) based on K2, and d) based on K3 representation of the hydraulic conductivity field at the MADE site. All three simulations were based on the dual-domain mass transfer model.


Z
Y
X
Concentration (pCi/mL)
300
100
50
25
10
5
a)
Z Axis (m)
60
55
-50
X Axis (m)
0
50
Y Axis (m)
0
50
100
150
200
250
b)
Z Axis
60
55
-50
X Axis
0
50
Y Axis
0
50
100
150
200
250
c)
Z Axis
60
55
-50
X Axis
0
50
Y Axis
0
50
100
150
200
250
d)
Z Axis
60
55
-50
X Axis
0
50
Y Axis
0
50
100
150
200
250

5.3. Dual-domain models

Results from dual-domain transport simulations (Fig. 7) based on the K2 and K3 conductivity representations show consistently low concentrations of tritium tracer at distances between 25 and 275 m away from the injection point, similar to observations from the MADE 2 experiment. Dual-domain simulations based on K1 representation are unable to reproduce this down gradient distribution of low tritium concentrations. Quantitative comparisons of the simulations to the observed tritium concentration ranged from $r=0.38$ to $r=0.64$. Simulations with mass transfer rate coefficients less than 0.0005 result in mass leaving the model domain during the simulation. Simulations with less than 90% of the initially injected mass remaining in the model domain were not considered to be viable models, since there is no evidence of significant mass leaving the model domain during the MADE 2 experiment. Simulations for both the K2 and K3 conductivity representations show roughness in the predicted 1D mass profile that is similar to the observed tritium profile.

5.4. Model comparisons

The transport simulations presented here are evaluated on the basis of statistical fit (r) and on qualitative comparisons of observed and predicted tritium plume characteristics such as location, amplitude, and width of peak concentrations in the integrated 1D mass profiles and the spreading of low tracer concentrations down gradient. Simulations with the best quantitative fit to the data typically have an r value >0.6, all of which are based on the dual-domain mass transfer model. These simulations also demonstrate a good qualitative fit to the observed mass profile (i.e., high peak and low concentration spreading in the 1D mass profile). In every simulation group (Figs. 6 and 7), the simulation based on the K2 conductivity representation resembles closely the simulation based on the K3 representation.

Simulations with the homogeneous layered K distribution (K1 representation) result in more peaked and fairly symmetrical Gaussian-type distributions of tracer mass. These simulations were unable to produce significant spreading of tracer more than 100 m down gradient from the injection point. Simulations that used the DC resistivity data to estimate hydraulic conductivity (K2 representation) produce results that match the observed mass distribution as closely as simulations based on the K3 representations that used only flowmeter measured hydraulic conductivity data (Figs. 6 and 7). This implies that K2 and K3 have similar 3D characteristics. Since K2 and K3 were obtained completely independent of each other, correlated by information from only one borehole flowmeter, the finding that K2 and K3 led to similar simulated plumes is quite significant.

In all conductivity representations, a longitudinal dispersivity value of 1m produced results that are most consistent with observations among the advection–dispersion models. In the dual-domain models, the optimal mass-transfer rate coefficient between mobile and immobile domains was $0.001\,\text{day}^{-1}$. A mass transfer rate coefficient of $0.0001\,\text{day}^{-1}$ tended to allow a substantial amount of tritium to escape the model domain after 328 days.

To this point, quantitative and qualitative comparisons have been made using the 1D profiles of tracer mass. Comparisons can also be made among the three-dimensional distributions of the three simulated plumes, each of which has the highest r value in their respective K groups with more than 90% simulated mass still remaining in the model domain at 328 days (simulations 1e, 2c, and 3d) (Fig. 8). Similar to the 1D comparisons, qualitative 3D comparisons also indicate that the simulation based on the K2 conductivity representation is able to predict the overall three-dimensional variation of tritium concentration as well as the K3 based conductivity simulation.

6. Summary

Groundwater flow and tracer transport at the MADE site was simulated by numerical models incorporating a DC resistivity derived hydraulic conductivity distribution. The simulated tracer mass profile agreed closely with the observed mass profile. The degree of agreement appears to be as good as that between the observed plume and the simulated plume that is based on an extensive amount of hydraulic conductivity data derived from borehole flowmeters. The geophysically derived K distribution presents an alternative to acquiring thousands of hydraulic conductivity measurements by borehole flowmeters or other methods in order to adequately characterize the three-dimensional flow field in heterogeneous aquifers. As has been demonstrated previously (e.g., Feehley et al., 2000) and in this paper, the advection–dispersion model and simple homogeneous layers of hydraulic conductivity are unable to fully represent transport in heterogeneous media. However, a dual-domain mass transfer model and properly chosen model parameters can reproduce the tritium experiment to a reasonable degree. The simulations presented here suggest that it is possible with one borehole flowmeter log of hydraulic conductivity and a 3D or pseudo 3D (parallel 2D lines) DC resistivity data to characterize the three-dimensional hydraulic conductivity field at a highly heterogeneous site to a reasonable degree in order to assess contaminant transport in practical field applications. It is noteworthy that the geophysical approach examined in this work may be useful in other aquifer systems under similar fluvial depositional environments, but the relationship between the hydraulic conductivity and DC resistivity is site specific and needs to be tested and determined at individual sites.

Acknowledgements

We thank Jerry McJunkin of Terraplus, Inc. for providing a scholarship to JCB that enabled us to conduct the resistivity research. BP-Amoco and the University of Alabama Department of Geological Sciences provided Summer Research Fellowships to JCB. We also thank the editor and three reviewers whose detailed and constructive comments have significantly improved this manuscript. This research was partially funded by NSF Grants EAR-0216520 and EAR-0003511.

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