A Forced Gradient Tracer Experiment in a Coastal Sandy Aquifer, Georgetown Site, South Carolina

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Abstract

A two-well tracer experiment was conducted in a coastal, sandy aquifer in South Carolina to investigate tracer migration in ground-water systems. Chloride tracer was injected into the aquifer under a steady flow condition created by continuous injection and withdrawal of ground water at an injection and a withdrawal well dipole separated by a distance of 5 meters. Breakthrough data were collected at several depths from two multilevel sampling wells, 1.5 meters apart, between the injection well and the withdrawal well.

A one-dimensional advection-dispersion model that considers the nonuniform velocity field of the two-well experiment was employed to estimate the hydrologic properties of the aquifer. The values of the porosity and dispersivity were estimated by fitting the model to the observed breakthrough data collected at three depths at one sampling well (Well A). These values were then used to predict the breakthroughs at the same depths in the other sampling well (Well B). A two-dimensional flow and transport model was also employed to simulate the tracer migration. Results of both one- and two-dimensional simulations show that these models fail to predict the tracer breakthrough at Well B using parameter values obtained from Well A.

The failure of the model to predict breakthroughs at Well B suggests that a three-dimensional characterization of aquifer heterogeneities and a three-dimensional modeling effort may be needed in order to capture the complex flow pattern in the aquifer.

Introduction

The hydrologic and chemical factors controlling the transport of natural organic matter (NOM) and colloidal particles in ground water is a subject of increasing interest because of the roles of these factors in ground-water pollution problems and bioremediation techniques (McCarthy and Zachara, 1989). In order to investigate these factors in the field, a forced-gradient tracer test is generally selected because the flow regime can be easily controlled. In a forced-gradient experiment, a steady-state flow field is established by pumping water out from the aquifer through a withdrawal well and injecting the water back into the aquifer through an injection well (Figure 1). Once the steady-state flow field is established, nonreactive and reactive tracers (such as chloride and NOM, respectively) are injected into the aquifer, and the tracer breakthroughs are then measured at sampling wells or at the withdrawal well. The breakthrough data of nonreactive tracers are used to determine the hydraulic parameters of the aquifer (i.e., hydraulic conductivity, porosity, and dispersivity). Once these values are determined, breakthrough data of reactive tracers such as NOM or colloids can be analyzed to estimate values of the parameters representing biochemical interactions between the tracer and the aquifer material.

Numerous forced-gradient, two-well experiments and related analyses have been conducted in the past few decades. For example, Hoopes and Harleman (1967) and Grove and Beetem (1971) investigated the movement of particles and their travel time in an injection-withdrawal well pair system. In particular, Hoopes and Harleman (1967) developed analytical solutions for describing tracer distribution in the two-well tracer experiment. They reported that the tracer concentration distribution at the withdrawal well during a continuous injection is mainly dominated by convection along different streamlines, and the effects of dispersion and diffusion are insignificant.

The use of two-well experiments for quantifying aquifer flow and transport parameters was demonstrated in the study by Pickens and Grisak (1981). Using two-well tracer experiments, they investigated the scale-dependent nature of aquifer dispersivity and concluded that the aquifer dispersivity increases with distance and depends on the aquifer hydraulic conductivity distribution and the distance between the two wells.

Molz et al. (1986) conducted a two-well tracer experiment in a fluvial terrace aquifer to investigate the feasibility of predicting tracer concentration distributions in the withdrawal well based on the vertical variation of hydraulic conductivity in the aquifer. Their study showed that the flow-averaged breakthrough data at the withdrawal well can be reasonably predicted if the hydraulic conductivity of each

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layer in the aquifer is specified. However, Molz et al. (1986) and Huyakorn et al. (1986a) reported that a fully three-dimensional solute transport model that assumes a perfectly stratified aquifer cannot reproduce the breakthrough data observed at different depths in a multilevel sampling well located between the injection and the withdrawal wells. They attributed the discrepancy to the inadequacy of the assumption of a perfectly stratified aquifer. In other words, variations in hydraulic conductivity at scales smaller than the layer have significant effects on the breakthrough data observed at the scale smaller than the thickness of the layer (Yeh, in press).

In this paper we describe a forced-gradient two-well experiment conducted in a coastal, sandy aquifer in Hobcaw Field at the Baruch Forest Science Institute, Georgetown, South Carolina. The experiment was conducted to analyze the migration of a nonreactive tracer (chloride). The major goals of the experiment were to provide the necessary hydrologic information to test the laboratory-derived understanding of the chemical processes involved in retention of NOM in the field, and to determine the relative importance of physical and hydrological factors on NOM transport in aquifers. It is our belief that a reliable characterization of hydraulic properties of the aquifer is necessary to accurately depict the velocity field that controls the transport of chemicals and contaminants. Once reliable velocity field is obtained, a correct interpretation of the parameters governing the chemical behaviors of NOM in the aquifer can be achieved.

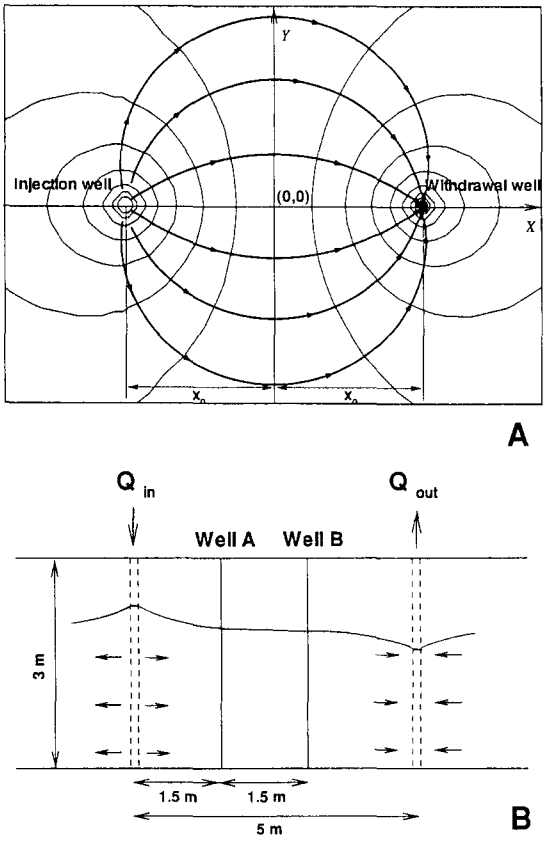

Fig. 1. Plan view (A) and cross section (B) of the two-well tracer test performed at Hobcaw Field.

Two-Well Tracer Experiment

The experiment was performed in the Summer of 1990 in an unconfined, sandy coastal plain aquifer (Williams and McCarthy, 1991). The aquifer is approximately 3 m thick, bounded by an impervious clay layer at the bottom, and exhibits distinct layering. The upper part of the aquifer consists of a layer of sand which contains iron oxide and some clay (approximately 9% by weight). Below this layer exists a zone of gleyed sand with 4% clay content, ranging in color from gray to pale olive gray. The deepest part of this aquifer is composed of a layer of coarse sand, ranging from 0.15 to 0.3 m thick, with a clay content less than 2%.

Figure 1 illustrates the location of the injection, withdrawal, and sampling wells. The distance between the injection and the withdrawal wells is 5 m; two multilevel sampling wells (wells A and B) are located at 1.5 and 3 m from the injection well, respectively. The injection and withdrawal wells (#10 PVC pipes of 0.05 m I.D.) are screened over the entire thickness of the saturated zone, capped at the bottom, and equipped with a seal at the top to aid forced injections. Each sampling well (0.0125 m diameter PVC pipes) has 11 sampling ports at 0.15 m intervals between 1.05 to 2.7 m below land surface. Each sampling port consists of an 0.05 m long section of 1 cm diameter PVC pipe with numerous 0.005 m diameter holes drilled along its length. These holes were covered with Nitex screen of mesh size equal to #10 diameter well screen. Each port was connected to a sampling device at the surface with an 0.008 m diameter teflon tubing. Samples were collected using a peristaltic pump at a flow rate of 50 ml/min.

The forced gradient was established by recirculating water from the withdrawal well to the injection well at an equal steady flow rate of 3.7 l/min. After several weeks of recirculation, the flow appeared to reach a steady-state condition. The hydraulic head was measured at the injection, withdrawal, and monitoring wells; the head difference between the injection and withdrawal wells was approximately 0.9 m. A regional flow gradient, approximately of 5×10^{-3}, was observed perpendicular to the well dipole. This gradient was small compared to the overall gradient induced by the forced injection and pumping dipole. After the steady state was reached, a potassium chloride (KCl) solution was added to previously reserved ground water and injected into the aquifer with an average chloride concentration of 140 mg/l during the first 23 hours. Then, the injection concentration was reduced to 30 mg/l for the remainder of the test. Figure 2a shows injected chloride concentration as a function of time. During the injection period, water pumped from the withdrawal well was discharged to a distant stream.

During the first 80 hours of the test, the chloride concentration was measured by a specific ion electrode at each sampling point every two or four hours. During the next 64 hours, measurements were taken every 10 or 14 hours. After 64 hours, samples were taken at longer intervals until the test ended at 12 days. Figures 2b through 2l depict the breakthrough data recorded at different depths from the two sampling wells. Descriptions of the experiment can also be found in Toran et al. (in press).

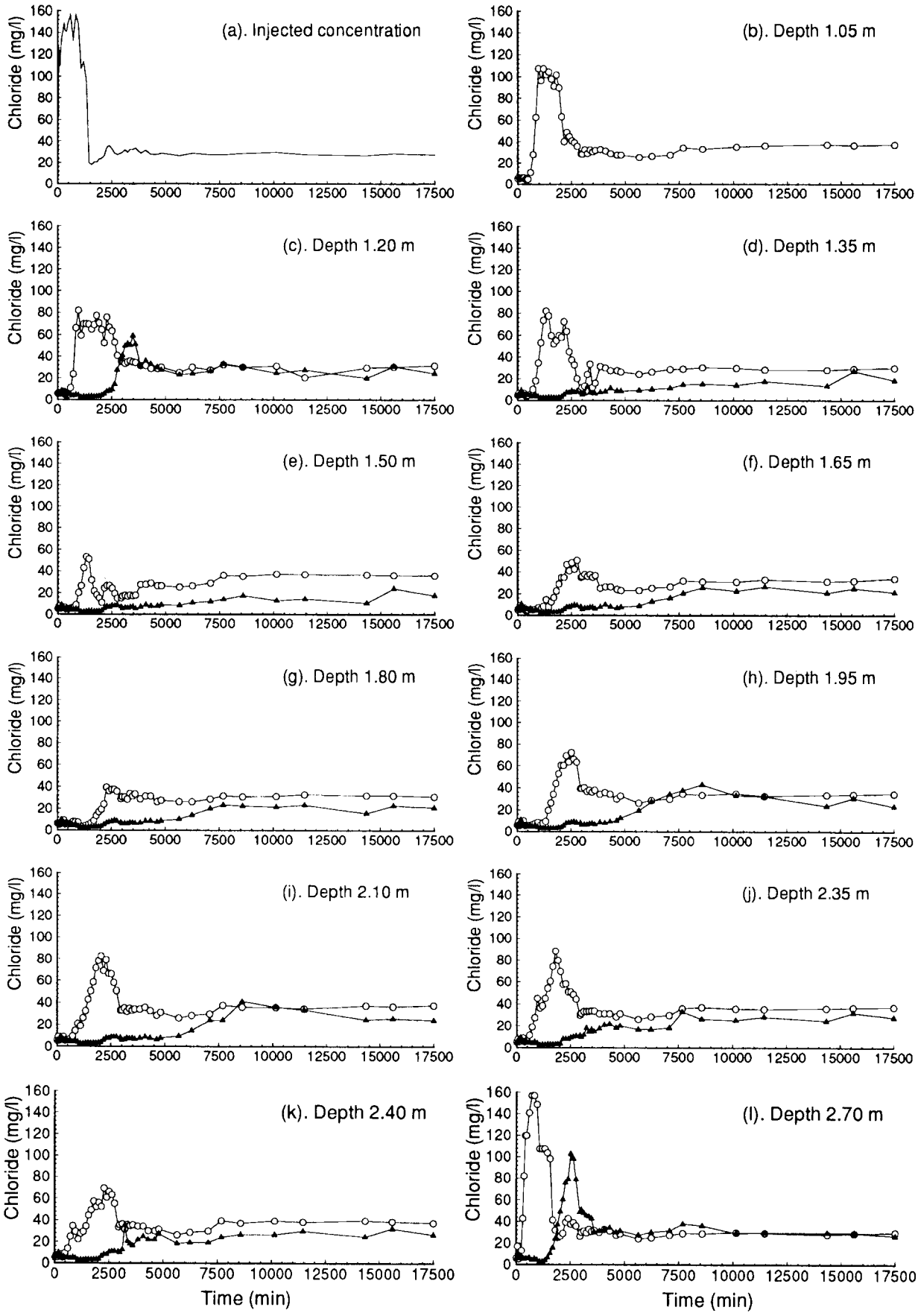

Fig. 2. a) Injected chloride concentration during the test; b) through l) Measured chloride breakthrough data at the 11 depths at Well A (circles) and Well B (triangles). Tracer concentration was not measured in Well B at 1.05 m depth because it became dewatered due to lowering of water table.

Parameter Estimation and One-Dimensional Simulation

To estimate the hydrologic properties, the aquifer was divided into 11 layers of constant thickness, corresponding to the location of the 11 sampling ports. Each layer was considered hydrologically homogeneous and isotropic. For each individual layer, a one-dimensional convection-dispersion model was used to simulate the migration of the tracer along the streamline between the injection and withdrawal wells. This model neglects the lateral mixing of tracer. The governing equation used by the model is given by:

$$\frac{\partial}{\partial s}\left(D(s)\frac{\partial C}{\partial s}\right) - v(s)\frac{\partial C}{\partial s} = \frac{\partial C}{\partial t} \qquad (1)$$

where C is the concentration in mass per unit volume; s is the distance along a streamline; v is the seepage velocity; D is the longitudinal hydrodynamic dispersion coefficient along a streamline; and t represents time. Since the flow field in the two-well test involves diverging and converging streamlines, the velocity in (1) varies with distance. Therefore, the longitudinal dispersion coefficient (the product of the dispersivity and the velocity) also changes with the distance. That is,

$$D(s) = \alpha\, v(s) \qquad (2)$$

where α is the dispersivity of the layer, assumed constant. By matching the calculated concentration [using (1) and (2)] to the measured breakthrough data, the dispersivity of the layer can be determined if the velocity along the streamline is known.

To determine the velocity field, the hydraulic gradient, which varies with distance, is considered constant over time and for each layer due to the steady-state flow assumption. The flow rate for each layer, Q(z), was estimated according to the procedure suggested by Güven et al. (1986):

$$Q(z) = \left(\frac{K_r}{K_{aver}}\right) \cdot Q_{aver} \qquad (3)$$

where K_r denotes the relative hydraulic conductivity, or conductivity normalized to the highest conductivity of all the layers (Pickens and Grisak, 1981). K_r is estimated by computing the relative arrival time of the peak concentration in each breakthrough data, i.e., as t_{min}/t_i, where t_i is the peak arrival time for layer i, and t_{min} is the minimum recorded peak arrival time. K_{aver} is the mean relative hydraulic conductivity of all the layers, and Q_{aver} is the mean flow rate per layer.

Table 1 shows the K_r values at Wells A and B. The vertical distribution of the values of K_r (Figure 3) is remarkably similar at both wells and consistent with the aquifer lithologic variations. Only two layers (identified by an asterisk in Figure 3) show a large difference in the K_r value. This difference probably can be attributed to the horizontal variation of the thickness of the layer as illustrated in the lithologic profile. Despite the difference, Q(z) was calculated using the relative hydraulic conductivities estimated at Well A ($K_{aver} = 0.53$, and $Q_{aver} = 0.34$ l/min).

Once the Q(z) values are known, the nonuniform seepage velocity components, v_x and v_y, for a homogeneous and isotropic aquifer with a fully penetrating well doublet operating at constant flow rate, may be estimated from (Huyakorn et al., 1986b):

$$v_x = -\frac{Q(z)}{2\pi\theta b}\left[\frac{x - x_o}{(x - x_o)^2 + y^2} - \frac{x + x_o}{(x + x_o)^2 + y^2}\right] \qquad (4)$$

$$v_y = -\frac{Q(z)y}{2\pi\theta b}\left[\frac{1}{(x - x_o)^2 + y^2} - \frac{1}{(x + x_o)^2 + y^2}\right]$$

Table 1. Breakthrough Data Analyses and Relative Hydraulic Conductivities

	Well A			Well B			
DEPTH	TIME	CONC	K_r	TIME	CONC	K_r	Q(z)
1.05	16	107	0.75	--	--	--	0.477
1.20	16	82	0.75	58	59	0.72	0.477
1.35	22	82	0.72	54	13	0.78	0.457
1.50	22	53	0.72	260	23	0.16	0.457
1.65	46	50	0.26	191	26	0.22	0.165
1.80	42	37	0.28	128	23	0.32	0.178
1.95	38	72	0.31	143	42	0.29	0.197
2.10	34	83	0.35	143	41	0.29	0.222
2.25	30	89	0.40	128	33	0.33	0.254
2.40	38	70	0.31	54	35	0.77	0.197
2.70	12	137	1.00	42	102	1.00	0.636

TIME: peak arrival time (hours)
CONC: chloride concentration at the peak (mg/l)
K: relative hydraulic conductivity (dimensionless)
Q(z): flow rate at depth z (l/min)

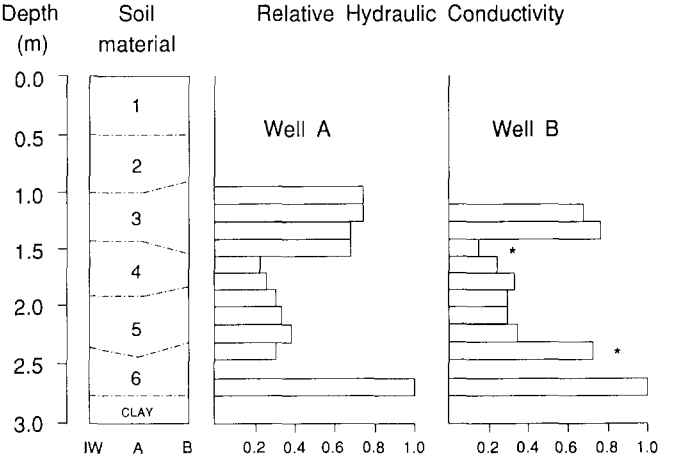

Fig. 3. Relative hydraulic conductivity distribution. Soil material column illustrates the horizon thickness at the injection well (IW), Well A (A) and Well B (B). Lithology description: 1: Brownish yellow fine sand with weak granular structure and fine and medium roots; 2: Yellowish brown loamy sand with weak medium subangular blocky structure, sand grains coated and bridged with clay, fine roots; 3: Yellowish brown loamy sand with weak medium granular structure, sand grains coated with clay, few fine roots; 4: Gray fine sand, single grained and highly gleyed; 5: Olive brown fine sand, single grained; 6: Yellowish brown medium-coarse sand, single grained and many clear quartz grains; material 6 is bounded by a massive gray clay layer at the bottom.

where Q(z) is the flow rate of each well; b is the aquifer thickness; θ is the porosity; and x_o is one-half the well spacing. The origin of the coordinate axes (x, y) is assumed to be at the center of the line joining the two wells; the x axis is oriented along this line (Figure 1). For the one-dimensional case, where Wells A and B are aligned with the injection and the withdrawal wells, the terms involving the y-coordinate are discarded.

Using the calculated velocity distribution, a finite-element method using linear basis functions was employed to solve equation (1) numerically. In order to consider a nonuniform velocity field, velocity between nodes is weighted by the linear shape function. The numerical results were validated by comparison with available analytical solutions for the uniform and nonuniform velocity cases (Hoopes and Harleman, 1967). The finite-element model was then used to estimate the dispersivity and porosity values by adjusting these parameters until it reproduced the observed breakthrough data at Well A. The goodness-of-fit was determined by visual judgment. To avoid numerical oscillations in the numerical solution, a Peclet number [$Pe = v(s)\,\Delta l/D$, where Δl is the element length] smaller than 2 and a Courant number [$Cr = v(s)\,\Delta t/\Delta l$, where Δt is the time step size] smaller than 1 were chosen (Huyakorn and Pinder, 1983). A constant concentration boundary condition was defined at the injection well, taking into account the chloride input variations shown in Figure 2a.

For the sake of simplicity, layers at 1.20, 2.25, and 2.70 m depth were chosen to calibrate the transport equation. These layers represent each of the three different soil bands defined by the K_r values (Figure 3). Table 2 tabulates the calibrated values of porosity and dispersivity. Figure 4 plots the simulated breakthrough curves versus field data at the three layers at Well A. In general, the simulated and observed breakthroughs are in good agreement. The steep shape of the ascending and descending branches of the breakthrough curves at 1.20 and 2.70 m depth suggests advection-dominated transport, which justifies the small dispersivity values obtained for these layers. The simulated results with these values, however, overestimate the low peak concentration recorded at depth 1.20 m. In contrast, the relatively large spread of the breakthrough data at the 2.25 m depth was simulated by using a larger dispersivity value.

Based on the assumption of homogeneity within each layer, the estimated values of porosity and dispersivity were expected to mimic the breakthrough data at Well B. Therefore, the model was used with the same velocity field, dispersivity, and porosity values obtained from the previous calibration to predict the breakthrough data at Well B. The result is illustrated in Figure 4. This figure shows that the agreement between the simulated and observed data is poor. The lack of agreement could be attributed to the disturbance of soils around Well B caused by installation, or to the sampling procedures. However, Wells A and B were installed and sampled at the same time, using the same techniques. Furthermore, the good agreement in the vertical spatial pattern of the K_r values obtained at both sampling wells (Figure 3) appears to contradict this speculation.

Table 2. Values of Porosity and Dispersivity Obtained by the Numerical Solutions

	1-D simulation		2-D simulation		
Depth	θ	α	θ	α	K
1.20	0.60	0.10	0.27	0.07	8.87×10^{-5}
2.25	0.50	0.25	0.35	0.20	4.71×10^{-5}
2.70	0.25	0.05	0.12	0.05	1.19×10^{-4}

θ: porosity
α: dispersivity (m)
K: hydraulic conductivity (m/s)

Two-Dimensional Simulations

To improve the results of one-dimensional simulation and to obtain the spatial distribution of the plume in the horizontal plane, a two-dimensional convection-dispersion model (Konikow and Bredehoeft, 1978) was used. This model considers both longitudinal and horizontal transverse dispersion, and it solves the flow equation using a finite-differences scheme, and the transport equation by the method of characteristics to avoid numerical dispersion and oscillation.

In the following two-dimensional simulations, the aquifer was assumed to be perfectly stratified and homogeneous, layers are considered to be isotropic with respect to hydraulic conductivity, and transverse dispersivity is one-third of longitudinal dispersivity (Bear, 1972). In addition to the dispersivity and porosity values, the two-dimensional simulations require absolute hydraulic conductivity values as input. These values were obtained by adjusting initial guessed values until the simulated and the observed head difference between the injection and withdrawal wells were in good agreement. Once the conductivity values were estimated, the values of porosity and dispersivity were calibrated to fit the breakthrough data recorded at Well A.

The estimated values for hydraulic conductivity, porosity, and longitudinal dispersivity for the two-dimensional simulation are presented in Table 2. These values provided a fit very similar to the one obtained in the one-dimensional simulation (Figure 4). The porosity values obtained in two-dimensional simulations are approximately one-half of those in the one-dimensional cases, however. As a result, the calculated velocities between the two wells are notably larger than those in the one-dimensional case. This discrepancy probably can be attributed to the effect of lateral dispersion in two-dimensional simulations. It is also possible that the assumptions defined for each particular model may play an important role in these differences. The two-dimensional model appears to be more realistic, but the porosity obtained is close to, or lower than, the lower limit of porosities for unconsolidated materials found in the literature (Davis, 1969). These low values of porosity may reflect the existence of dead-end pores and preferential flow paths. However, without direct measurements of the hydraulic properties, the representativeness of the estimated porosity values remains unknown.

Even though horizontal transverse dispersion is considered in the two-dimensional model, the same difficulty

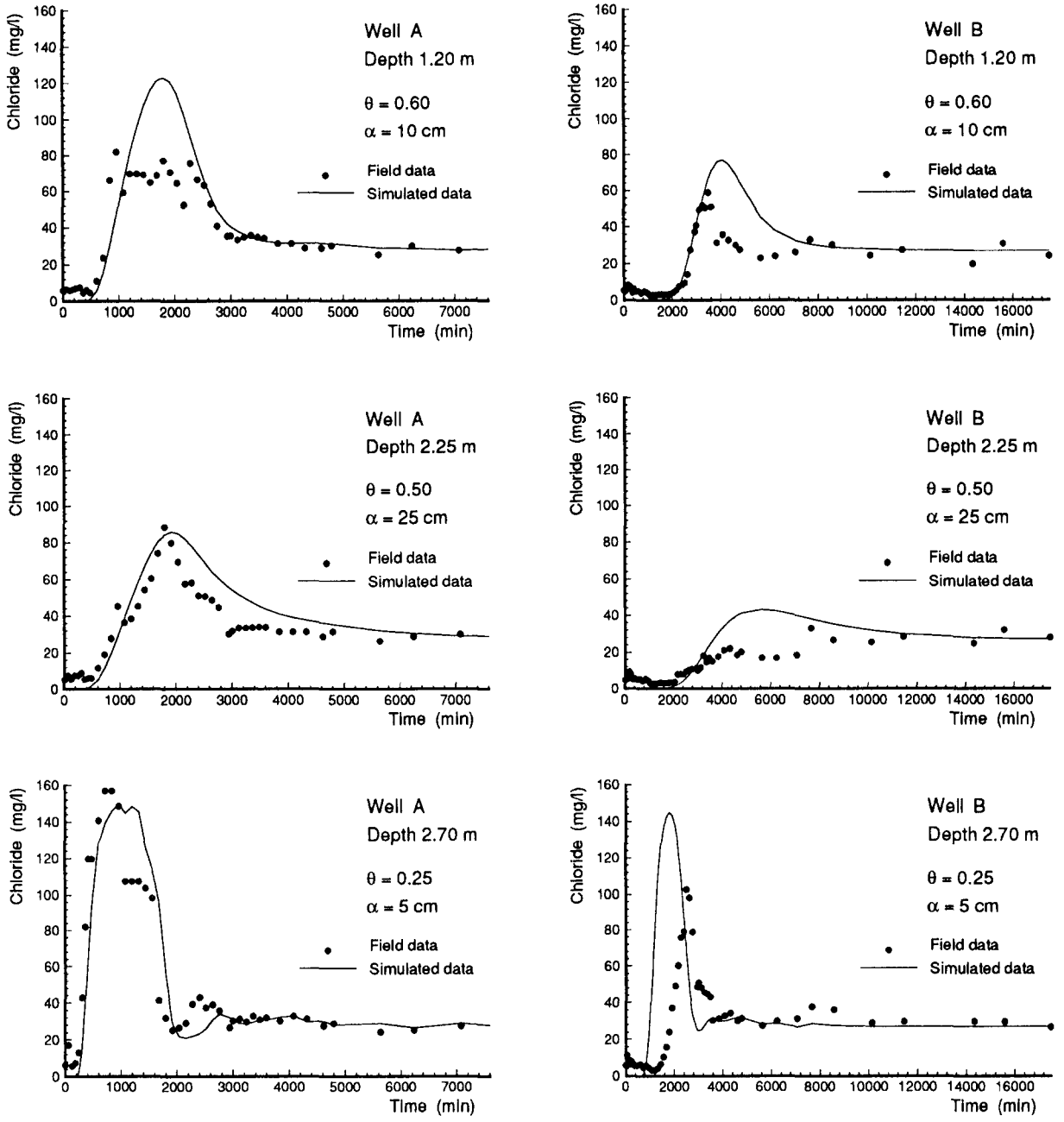

Fig. 4. Measured (dots) and simulated (solid) chloride breakthrough curves using a one-dimensional model at observation wells A and B.

was encountered as in the one-dimensional model: failure to reproduce the breakthrough data at Well B (Figure 4). Similar difficulties in prediction of breakthrough data recorded at various depths of an aquifer were also reported by Molz et al. (1986) and Huyakorn et al. (1986). These difficulties are analogous to the problems of predicting breakthrough data in a single pore of a soil column using a classical convection-dispersion equation [i.e., equation (1)]. The equation is based on the assumption of volume average, i.e., the predicted concentration represents the average concentration over many pores, instead of the concentration in a single pore. More precisely, the scale of observation in a single pore is inconsistent with the scale of the volume over which the process is averaged in the governing equation. This inconsistency is the so-called scale problem (Yeh, in press). Indeed, Molz et al. (1986) reported successful predictions of breakthrough data collected in a withdrawal well which is screened over the entire thickness of the aquifer. This scale problem leads us to believe that a detailed three-dimensional site characterization and three-dimensional flow and transport simulations that consider the heterogeneity of the field site are necessary for predicting the breakthrough data at each multilevel sampling port.

Summary and Conclusions

A two-well tracer test was used to investigate the hydraulic and transport properties of a sandy aquifer. The breakthrough data of a conservative tracer were used to estimate the properties based on one- and two-dimensional models, assuming perfectly horizontal stratification and

homogeneity. Although the breakthrough data can be reproduced satisfactorily in one of the sampling wells, different values of porosity must be used in each model. More importantly, the chloride breakthrough data at Well B (1.5 meters away from Well A) cannot be successfully predicted by any of the models, suggesting that the assumption of homogeneity is inadequate.

Failure to reproduce the breakthrough data at Well B indicates that parameter estimation based on breakthrough data at a single point is insufficient to define the hydrologic properties of the aquifer due to spatial heterogeneity. As a result, predictions of transport of conservative tracers based on the estimated parameter have large uncertainties. These difficulties raise serious questions about our ability to characterize and predict reactive chemical transport in field conditions.

To resolve these problems, a three-dimensional site characterization using small-scale measurements, and a fully three-dimensional model incorporating detailed hydraulic conductivity variations is recommended. It is our belief that such a detailed site characterization and simulation will provide a more accurate description of the flow field of the experiment site. The migration of a conservative tracer can thus be better predicted, and the uncertainty due to spatial variability of hydraulic parameter can be reduced. As a result, a valid and reliable interpretation of the chemical processes involved in colloid or other reactive solute transport in the field can be achieved.

Acknowledgments

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