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One-Dimensional Solute Transport in Porous Media With Partial Well-to-Well Recirculation: Application to Field Experiments

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A solute transport model incorporating well-to-well recirculation was developed to facilitate the interpretation of pilot-scale field experiments conducted for the evaluation of a test zone chosen for in situ restoration studies of contaminated aquifers, where flow was induced by recirculation of the extracted fluid. A semianalytical and an approximate analytical solution were derived to the one-dimensional advection-dispersion equation for a semi-infinite medium under local equilibrium conditions, with a flux-type inlet boundary condition accounting for solute recirculation between the extraction-injection well pair. Solutions were obtained by taking Laplace transforms to the equations with respect to time and space. The semianalytical solution is presented in Laplace domain and requires numerical inversion, while the approximate analytical solution is given in terms of a series of simple nested convolution integrals which are easily determined by numerical integration techniques. The applicability of the well-to-well recirculation model is limited to field situations where the actual flow field is one dimensional or where an induced flow field is obtained such that the streamlines in the neighborhood of the monitoring wells are nearly parallel. However, the model is fully applicable to studies of solute transport through packed columns with recirculation under controlled laboratory conditions. The model successfully simulated tracer breakthrough responses at a field solute transport study, where an induced flow field superimposed on the natural gradient within the confined aquifer was created by a well pair with extraction to injection rates of 10: 1.4.

INTRODUCTION

Solute transport through porous media is of practical importance in diverse applications: saltwater intrusion of coastal aquifers, tertiary oil recovery processes, and movement of adsorbing or reacting species in packed beds or in aquifers. Mathematical modeling of transport processes has increasingly captured the attention of many researchers, particularly hydrogeologists and environmental engineers, because of the public concern and the widespread attention on the disposal, movement, and fate of toxic contaminants in natural subsurface systems.

The transport of nonreactive solutes through homogeneous porous media consisting of impermeable grains has been commonly characterized by the classical advection-dispersion equation, which is based on the empirical relation of Fick's diffusion law [*Fried and Combarnous*, 1971; *Bear*, 1972]. For sorbing solutes the advection-dispersion equation has been modified to incorporate the effects of adsorption [*Hashimoto et al.*, 1964; *Lindstrom et al.*, 1967], and hysteresis [*van Genuchten et al.*, 1974]. However, in order to simulate the asymmetry and tailing of breakthrough curves observed in several experimental studies of solute transport, models have been developed to account for solute exchange between zones of mobile and completely mixed immobile water [*Deans*, 1963; *Coats and Smith*, 1964; *van Genuchten and Wierenga*, 1976] and physical nonequilibrium models that incorporate solute transfer by the second law of diffusion into immobile regions of various geometries [*Rasmuson and Neretnieks*, 1980; *Goltz and Roberts*, 1986*a*; *van Genuchten and Dalton*, 1986]. The majority of the mathematical models in current use for solute transport with sorption processes are based on chemical equilibrium isotherms rather than on kinetic sorption relationships because of their computational simplicity. However, it must be pointed out that the validity of the local chemical equilibrium assumption has been questioned in studies of sorbing solute transport through laboratory columns [*James and Rubin*, 1979; *Nkedi-Kizza et al.*, 1983; *Miller and Weber*, 1986] and through aquifers [*Pickens et al.*, 1981; *Goltz and Roberts*, 1986*b*; *Roberts et al.*, 1986].

There are certain cases where direct application of the existing analytical solutions to solute transport models is not adequate. For example, in a demonstration of in situ restoration of contaminated aquifers a flow field is induced between an injection-extraction well pair, where chemicals of interest are introduced into a fraction of the extracted fluid which is reinjected [*Semprini et al.*, 1987]. In geothermal fields it is common to reinject thermally spent hydrothermal brines, which contain high levels of environmentally hazardous toxic minerals and cannot be discharged as surface waters [*Horne*, 1985; *Chrysikopoulos and Kruger*, 1986]. Clearly, in such systems the movement of injected solutes cannot be simulated accurately without taking into account the feedback due to recirculation.

This work extends the collection of solute transport models by presenting solutions to one-dimensional transport through porous media under local equilibrium conditions and solute recirculation between the extraction-injection well pair. The solutions are developed for a flux-type inlet boundary condition in a semi-infinite medium. Although one-dimensional models may not be adequate for every field situation, this particular model provides a starting point for investigating the effects of well-to-well recirculation. Furthermore, for one-dimensional models, analytical or semianalytical solutions are most likely obtainable. When these solutions are applicable, they are more efficient and accurate computations than the purely numerical solutions of multidimensional models. The model is applied to an actual field situation where well-to-well recirculation occurs in an induced flow field superimposed on the natural gradient of the

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confined aquifer with extraction to injection rates of 10: 1.4, under broad solute pulse injection conditions.

MODEL DEVELOPMENT

The transport of a sorbing solute through one-dimensional porous media under steady state flow conditions is governed by the following partial differential equation [*Lapidus and Amundson*, 1952]:

$$\frac{\partial C(t, x)}{\partial t} + \frac{\rho}{\theta}\frac{\partial C^*(t, x)}{\partial t} = D\frac{\partial^2 C(t, x)}{\partial x^2} - U\frac{\partial C(t, x)}{\partial x} \quad (1)$$

where C is the liquid phase solute concentration (M/L^3), C^* is the solid phase concentration of the adsorbed solute (M/M), D is the hydrodynamic dispersion coefficient (L^2/t), U is the average interstitial fluid velocity (L/t), x is the spatial coordinate in the direction of flow (L), t is the time (t), ρ is the bulk density of the solid matrix (M/L^3), and θ is the porosity (L^3/L^3). For linear, reversible, instantaneous sorption the equilibrium relationship between the solute substance in the aqueous and solid phases is given by

$$C^*(t, x) = K_d C(t, x) \quad (2)$$

where K_d is the partition or distribution coefficient (L^3/M). The distribution coefficient is a measure of solute retention by the solid and is expressed as the ratio of solute concentration on the adsorbent to solute concentration in solution. Combining equations (1) and (2) leads to

$$R\frac{\partial C(t, x)}{\partial t} = D\frac{\partial^2 C(t, x)}{\partial x^2} - U\frac{\partial C(t, x)}{\partial x} \quad (3)$$

where the dimensionless variable R is the retardation factor defined as

$$R = 1 + (\rho/\theta)K_d \quad (4)$$

For a semi-infinite system and pulse input conditions that take into account the effect of solute recirculation, the appropriate initial and boundary conditions are

$$C(0, x) = 0 \quad (5a)$$

$$\begin{aligned} -D\frac{\partial C(t, 0)}{\partial x} + UC(t, 0) &= U[C_p + qC(t, l)] \quad 0 < t \le t_p \\ -D\frac{\partial C(t, 0)}{\partial x} + UC(t, 0) &= qUC(t, l) \quad t > t_p \end{aligned} \quad (5b)$$

$$\frac{\partial C(t, \infty)}{\partial x} = 0 \quad (5c)$$

where C_p is the pulse-type injection concentration (M/L^3), and t_p is the duration of the solute pulse (t). The initial condition (5a) establishes that there is no initial solute concentration within the one-dimensional porous medium. The third- or flux-type boundary condition (5b) for pulse injection implies concentration discontinuity at the inlet and leads to material balance conservation [*Brigham*, 1974; *Choi and Perlmutter*, 1976; *Kreft and Zuber*, 1978; *Parker and van Genuchten*, 1984]. The upstream boundary condition (5b) includes, on the right-hand side, the term of $qC(t, l)$, where $C(t, l)$ is the solute concentration at the extraction location l, and q is the fraction of the recirculating solute mass ($0 \le q \le 1$). This term accounts for solute recirculation between the extraction-injection locations by adjusting instantaneously the inlet concentration in proportion to the solute concentration at the exit. The downstream boundary condition (5c) preserves concentration continuity for a semi-infinite system.

Semianalytical Solution

The solution to (3), subject to initial and boundary conditions described by equations (5a)–(5c) is obtained by the methods of *Lindstrom and Boersma* [1971] and *Chrysikopoulos et al.* [1990]. Taking the Laplace transforms of these equations with respect to the time variable t and the space variable x leads to the following set of algebraic equations:

$$R[s\bar{C}(s, \gamma) - \bar{C}(0, \gamma)] = D[\gamma^2\bar{C}(s, \gamma) - \gamma\bar{C}(s, 0) - \bar{C}_x(s, 0)] - U[\gamma\bar{C}(s, \gamma) - \bar{C}(s, 0)] \quad (6a)$$

$$\bar{C}(0, \gamma) = 0 \quad (6b)$$

$$-D\bar{C}_x(s, 0) + U\bar{C}(s, 0) = U[C_p/s + q\bar{C}(s, l)] \quad (6c)$$

$$\bar{C}_x(s, \infty) = 0 \quad (6d)$$

where

$$\bar{C}(s, \gamma) = \int_0^\infty \int_0^\infty C(t, x)e^{-st}e^{-\gamma x}\, dt\, dx$$

the tilde signifies Laplace transform, and s, γ are the Laplace domain time and space variables, respectively. Substituting initial condition (6b) into (6a), employing boundary condition (6c), and solving for $\bar{C}(s, \gamma)$ yields

$$\bar{C}(s, \gamma) = \frac{\gamma\bar{C}(s, 0) - (U/D)[C_p/s + q\bar{C}(s, l)]}{(\gamma + M - N)(\gamma + M + N)} \quad (7)$$

where

$$M = -U/2D \quad (8)$$

$$N = [Rs/D + U^2/(4D^2)]^{1/2} \quad (9)$$

Using Laplace transforms from the tabulation of *Roberts and Kaufman* [1966], the inverse of (7) with respect to γ is determined to be

$$\bar{C}(s, x) = \bar{C}(s, 0)\frac{-(M - N)e^{-(M - N)x} + (M + N)e^{-(M + N)x}}{2N} - \frac{U}{D}\left[\frac{C_p}{s} + q\bar{C}(s, l)\right]\frac{e^{-(M - N)x} - e^{-(M + N)x}}{2N} \quad (10)$$

Applying boundary condition (6d) in (10) and taking the limit $x \to \infty$, $\bar{C}(s, 0)$ is evaluated to be

$$\bar{C}(s, 0) = \frac{-U}{D(M - N)}\left[\frac{C_p}{s} + q\bar{C}(s, l)\right] \quad (11)$$

and upon substitution into (10) yields

$$\bar{C}(s, x) = -\frac{U}{D}\left[\frac{C_p}{s} + q\bar{C}(s, l)\right]\frac{e^{-(M + N)x}}{(M - N)} \quad (12)$$

Setting $x = l$ in equation (12), $\bar{C}(s, l)$ is evaluated to be

$$\bar{C}(s, l) = -\frac{[UC_p/(sD)][e^{-(M+N)l}/(M-N)]}{1 + (qU/D)[e^{-(M+N)l}/(M-N)]} \tag{13}$$

Substituting (13) into (12) leads to

$$\bar{C}(s, x) = -\frac{UC_p}{sD}\frac{e^{-(M+N)x}}{(M-N)}\left[1\Big/\left(1 - \frac{qU}{D}\frac{e^{-(M+N)l}}{(N-M)}\right)\right] \tag{14}$$

Analytical inversion of (14) with respect to s is too difficult to obtain, and numerical inversion of the Laplace transform by techniques such as the Stehfest algorithm [*Stehfest*, 1970], Fourier series approximations [*Dubner and Abate*, 1968; *Crump*, 1976] are required. Therefore the semianalytical solution in the Laplace domain is given by

$$\begin{aligned} C(t, x) &= \Omega(t, x) && 0 < t \le t_p \\ C(t, x) &= \Omega(t, x) - \Omega(t - t_p, x) && t > t_p \end{aligned} \tag{15a}$$

where

$$\Omega(t, x) = L^{-1}\{\bar{C}(s, x)\} \tag{15b}$$

and L^{-1} is the Laplace inverse operator.

Approximate Analytical Solution

The expression (14) can be reduced by a good approximation to a format for which analytical inversion is achievable. For the case where

$$\left(\frac{qU}{D}\right)\frac{e^{-(M+N)l}}{N-M} \ll 1 \tag{16}$$

the Maclaurin approximation $1/(1 - x) \approx 1 + x + x^2 + x^3 \cdots$ is employed to simplify (14) as follows:

$$\bar{C}(s, x) = \sum_{m=1}^{\infty}(-1)^m \frac{q^{m-1}C_p}{s} \cdot \left(\frac{U}{D}\right)^m \frac{\exp\{-(M+N)[x + (m-1)l]\}}{(M-N)^m} \tag{17}$$

Resubstituting equations (8) and (9) into (17), inversion from Laplace time variable s to real time t is straightforward, and all necessary transforms can be found in the tabulation of *Roberts and Kaufman* [1966]. The Laplace inversion of the first term, $A(t, x)$, on the right-hand side of equation (17) yields the well-known solution to the one-dimensional advection-dispersion solute transport model with third-type boundary condition without recirculation [*Lindstrom et al.*, 1967; *Gershon and Nir*, 1969]:

$$A(t, x) = \frac{C_p}{2}\operatorname{erfc}\left[\frac{Rx - Ut}{2(DRt)^{1/2}}\right] + C_p\left(\frac{U^2t}{\pi DR}\right)^{1/2}\exp\left[-\frac{(Rx - Ut)^2}{4DRt}\right] - \frac{C_p}{2}\left(1 + \frac{Ux}{D} + \frac{U^2t}{DR}\right)\exp\left[\frac{Ux}{D}\right] \cdot \operatorname{erfc}\left[\frac{Rx + Ut}{2(DRt)^{1/2}}\right] \tag{18}$$

The Laplace inversion of the second term, $B(t, x)$, on the right-hand side of equation (17) is given by

$$B(t, x) = L^{-1}\left\{-\frac{C_pU}{sD}\frac{e^{-(M+N)x}}{(M-N)}\right\}L^{-1}\left\{-\frac{qU}{D}\frac{e^{-(M+N)l}}{(M-N)}\right\} = A(t, x)*G(t, l) = \int_0^t A(\tau, x)G(t - \tau, l)\, d\tau \tag{19}$$

where the star signifies convolution, $A(t, x)$ is as defined in (18), and $G(s, l)$ is given by

$$G(t, l) = q\left(\frac{U^2}{\pi DRt}\right)^{1/2}\exp\left[-\frac{(Rl - Ut)^2}{4DRt}\right] - \left(\frac{qU^2}{2DR}\right)\exp\left[\frac{Ul}{D}\right]\operatorname{erfc}\left[\frac{Rl + Ut}{2(DRt)^{1/2}}\right] \tag{20}$$

The Laplace inversion of the third term, $\Gamma(t, x)$, on the right-hand side of equation (17) is given by

$$\Gamma(t, x) = B(t, x)*G(t, l) = \int_0^t B(\tau, x)G(t - \tau, l)\, d\tau \tag{21}$$

All other terms in the series (17) are evaluated in a similar fashion. Therefore the approximate analytical solution of the proposed one-dimensional solute transport model with well-to-well recirculation in the real time and space domain is

$$\begin{aligned} C(t, x) &= \Phi(t, x) && 0 < t \le t_p \\ C(t, x) &= \Phi(t, x) - \Phi(t - t_p, x) && t > t_p \end{aligned} \tag{22a}$$

where

$$\Phi(t, x) = A(t, x) + \sum_{m=1}^{\infty}\alpha_m(t, x)*G(t, l) \tag{22b}$$

$$\alpha_1(t, x) = A(t, x) \tag{22c}$$

$$\alpha_m(t, x) = \alpha_{m-1}(t, x)*G(t, l) \qquad m \ge 2 \tag{22d}$$

and the nested convolution integrals are easily determined by numerical integration techniques.

The evaluation of condition (16) is not straightforward since the parameter N incorporates time in Laplace domain. However, due to the exponential decay term, the approximation is always justified for large l. Figure 1 shows plots of dimensionless concentration versus time for the approximate analytical solution (22), the semianalytical solution (15), and the case of no recirculation ($q = 0$). The semianalytical solution was obtained by numerical inversion of the Laplace transform utilizing the Stehfest algorithm [*Stehfest*, 1970], while the convolution integrals of the approximate analytical solution were evaluated by Simpson's rule. For this illustrative comparison only the first three terms of the infinite series (22*b*) were taken into account. The predictions of the analytical and semianalytical solutions are indistinguishable. For $q \ll 1$ the approximate analytical solution can be utilized efficiently with just a few terms of the infinite

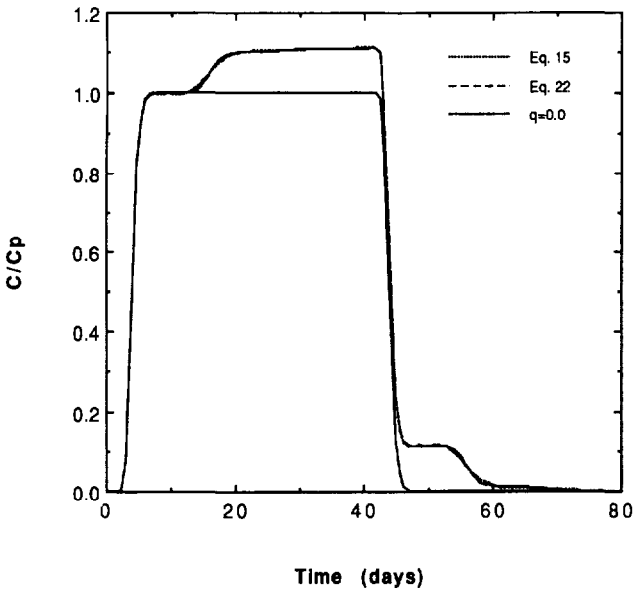

Fig. 1. Comparison of the approximate analytical, semianalytical, and case of no recirculation solutions: $U = 0.5$ m/d, $D = 0.02$ m^2/d, $R = 1$, $C_p = 1.0$ mg/L, $x = 2.0$ m, $l = 6.0$ m, $t_p = 40.0$ days, and $q = 0.1$.

series, because at late stages of a broad pulse injection the breakthrough concentration increases only very slowly. However, for $q \sim 1$ the number of the required summation terms in the infinite series is determined by the number of injected fluid recirculations or equivalently the number of pore volumes passing through the system during the experimental period. For example, if $q = 1$, the breakthrough concentration at the end of k fluid recirculations is approximately kC_p.

Parameter Estimation Methodology

The model developed above generally contains four parameters, namely, the retardation factor, the dispersion coefficient, the fluid velocity, and the fraction of the recirculating solute mass. In applying the model to laboratory or field data it is necessary to best estimate these parameters and to quantify their uncertainty. There are several approaches available for parameter determination. Here the nonlinear least squares regression method has been adopted.

In general, the objective of the nonlinear least squares method is to obtain estimates of the model parameters which minimize the residual sum of squares between simulated and observed data. The objective function may be written as

$$S(\hat{\mathbf{b}}) = [\mathbf{y} - \mathbf{g}(\mathbf{u}, \hat{\mathbf{b}})]^T[\mathbf{y} - \mathbf{g}(\mathbf{u}, \hat{\mathbf{b}})] \quad (23)$$

where $\mathbf{y} = \mathbf{g}(\mathbf{u}, \mathbf{b}) + \mathbf{e}$ is an $n \times 1$ observation vector, $\mathbf{g}$ is an $n \times 1$ vector of model simulated data, $\mathbf{u}$ is a vector of independent variables (time, space locations), $\mathbf{b}$ is an $p \times 1$ vector of the true but unknown parameters, $\mathbf{e}$ is an $n \times 1$ random vector with zero mean and known covariance matrix, and the circumflex denotes an estimate.

In this study the Standards Times Series and Regression Package (STARPAC) [*Donaldson and Tryon*, 1983] was used for parameter estimation. STARPAC includes an adaptive nonlinear least squares algorithm developed by *Dennis et al.* [1981]. This algorithm adaptively decides when to use the computationally expensive second-order part of the least squares Hessian, which accounts for its reliability and efficiency when the residuals are large or the model is highly nonlinear.

Quantifying the uncertainty of the estimated nonlinear parameters by approximate 95% confidence intervals, which are based on a single-variate Student's t distribution assuming normally distributed parameter estimates, may be criticized because these limits do not yield joint confidence regions. Joint confidence intervals or confidence regions are preferable. However, although the concept of confidence region construction is intuitively simple, it can lead to considerable difficulties. The results of a Monte Carlo study on approximate confidence region evaluations for nonlinear least squares parameter estimates conducted by *Donaldson and Schnabel* [1987] have shown that the simple and most frequently used linearization methods are often grossly underestimating confidence regions. On the other hand, the likelihood and lack-of-fit methods are considered reliable (see also *Vecchia and Cooley* [1987]). Since the utilization of such methods is a computationally demanding task, only the approximate 95% confidence intervals are presented in the following example.

Application to Field Experiments

Solute transport experiments were carried out at Moffett Naval Air Station, Mountain View, California, during the first phase of a field demonstration study for in situ restoration of aquifers contaminated with hydrocarbons [*Semprini et al.*, 1987]. Bromide was injected as a conservative tracer into the subsurface test zone to characterize fluid residence times, dispersion coefficients, and degree of solute recovery.

The test zone is a shallow, confined aquifer approximately 1.2 m thick, 4.5 m below the ground surface. The aquifer material consists of fine- to coarse-grained sand and thin discontinuous lenses of gravel. Although several wells are installed on the field site that are designed to permit simultaneous experiments, the data used in this paper have been collected from the south subzone which consists of a fully penetrating injection-extraction well pair and three partially

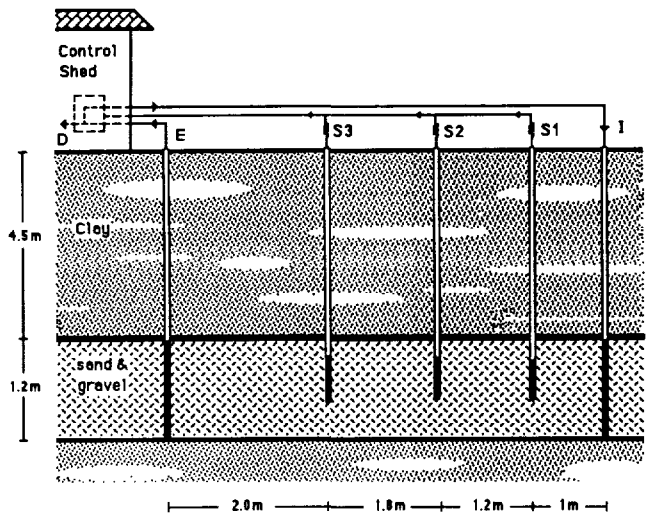

Fig. 2. Vertical cross section of the south test subzone: D, drain; E extract; I injection; and S1, S2, and S3, sampling wells.

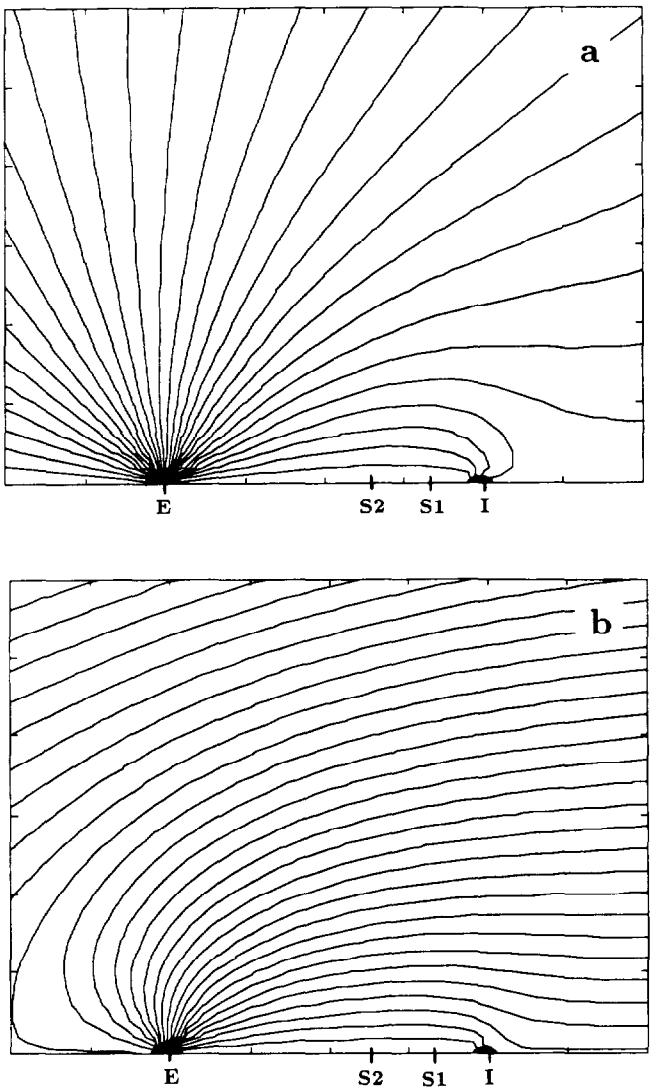

Fig. 3. (*a*) Streamlines for flow resulting from a well pair with extraction to injection rates of 10: 1.4. (*b*) Streamlines for flow resulting from a well pair with extraction to injection rates of 10: 1.4 and uniform regional flow.

penetrating monitoring wells (see Figure 2). The injection well is located 6 m south of the extraction well, whereas the monitoring wells are 1.0, 2.2, and 4.0 m from the injection well.

An induced flow field superimposing the natural gradient within the confined aquifer was created by extracting groundwater at a rate of 10 L/min and reinjecting a fraction of this fluid at a rate of 1.4 L/min. The bromide was introduced into the reinjected fluid as a broad pulse. The solute concentrations of the injected fluid, at the three monitoring wells and at the extraction well, were determined by an automated data acquisition system located at the field. Additional details of the field site and experimental and analytical procedures are given by *Semprini et al.* [1987].

Using potential flow theory and superposition of stream functions [*Strack*, 1989, p. 226], we determined that for the 10: 1.4 ratio of extraction to injection rates most of the flow is limited to within a narrow band between the two wells (see Figure 3*a*). As shown in Figure 3*b*, the width of the streamtube, which contains most of the flow, becomes even narrower in the presence of uniform regional flow from the injection to the extraction well. Furthermore, the streamlines in the neighborhood of the monitoring wells S1 and S2 are nearly parallel, implying that the velocity U is nearly constant in that subregion. Thus, although the actual flow is not exactly one dimensional, the one-dimensional model is a reasonable approximation. The boundary condition (5*c*) is introduced in the one-dimensional model to prevent loss of mass through dispersion upstream.

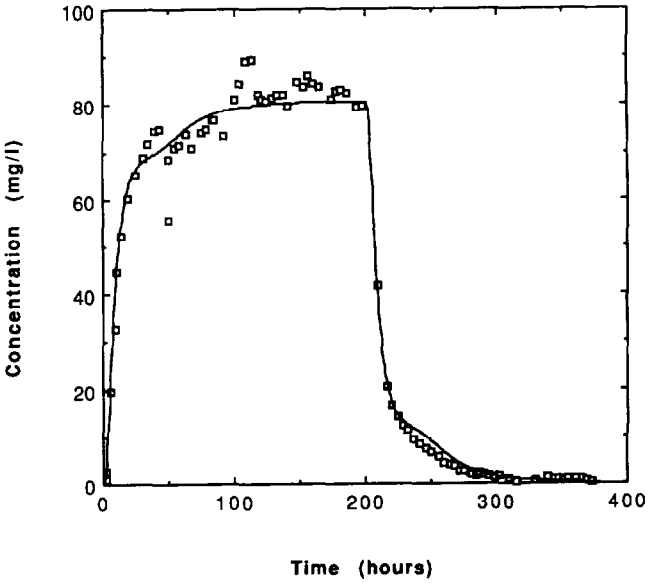

Fig. 4. Bromide concentration breakthrough data observed at S1 (squares) and simulated concentration history (solid curve).

The bromide breakthrough data observed at monitoring wells S1 (Figure 4) and S2 (Figure 5) from the experiment TRACER8 were used to validate the well-to-well recirculation solute transport model. For each data set the best estimates of the three unknown parameters U, D, and q were

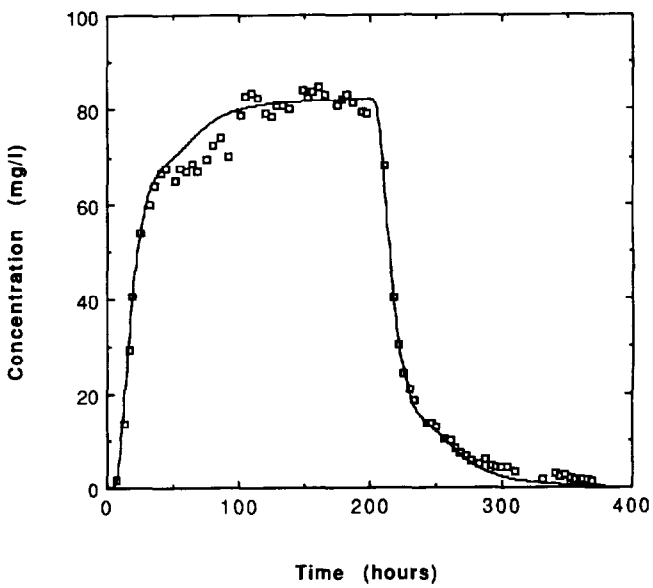

Fig. 5. Bromide concentration breakthrough data observed at S2 (squares) and simulated concentration history (solid curve).

TABLE 1. Estimated Transport Parameters for Bromide Breakthrough Data Observed at Sampling Locations S1 and S2

Parameter	Estimate	Standard Deviation	Approximate 95% Confidence Limits	
			Lower	Upper
		Monitoring Well S1		
U (m/h)	0.119	0.003	0.113	0.125
D (m^2/h)	0.032	0.004	0.024	0.040
q (−)	0.138	0.005	0.127	0.149
		Monitoring Well S2		
U (m/h)	0.123	0.002	0.120	0.127
D (m^2/h)	0.032	0.002	0.027	0.037
q (−)	0.154	0.005	0.145	0.164

obtained by the estimation methodology previously described. The fourth parameter of the model, R, was set equal to unity because bromide was considered as a conservative tracer. To improve convergence the parameter estimates were based only on the early breakthrough and the complete elution curves, excluding the middle portion of the observed responses (50–170 hours in Figures 4 and 5). The parameter estimates together with relevant statistics are given in Table 1. The relatively narrow 95% confidence limits of the estimated parameters, as well as the close agreement of the parameter estimates obtained for the two observed tracer concentration profiles, indicate that the model can adequately simulate the bromide transport and the solute recirculation effects, at least within the experimental subzone.

The actual bromide breakthrough responses observed at sampling locations S1 and S2 together with the model-simulated profiles are shown in Figures 4 and 5, respectively. Good agreement between the experimental data and the simulated concentration history is shown for both cases. A model which does not account for well-to-well recirculation would not have given such good predictions either at the middle portion of the observed response or at the late portion of the elution curve (see Figure 1). Clearly, the observed data incorporate some experimental error, caused mainly by slight inconsistencies in daily calibrations of the analytical apparatus. Such variations in the observed data cannot be simulated. Furthermore, the one-dimensional, well-to-well recirculation solute transport model developed herein cannot account for the inhomogeneities and the three-dimensional nature of the real environment. Nonetheless, there is a remarkably good agreement between the parameter estimates for U and D at the two monitoring wells, S1 and S2, as seen in Table 1. These parameters should be interpreted as "effective" ones. Additional simulations of tracer breakthrough field responses are given by *Chrysikopoulos and Roberts* [1989].

SUMMARY

A semianalytical and an approximate analytical solution to the one-dimensional advection-dispersion transport model accounting for well-to-well recirculation have been presented. Solutions are given for a flux-type inlet boundary condition and semi-infinite medium. Sorption is assumed to be governed by a linear equilibrium isotherm. The model is fully applicable to studies of solute transport through packed columns under controlled laboratory conditions. The applicability of this model to well-to-well recirculation is limited to situations where the actual flow field is approximately one dimensional. This is the case when the extraction rate greatly exceeds the injection rate, as in the situation presented here. The flow could not be treated as one dimensional if the injection and extraction rates were nearly equal.

Bromide breakthrough concentration profiles, obtained from the transport studies at the Moffett site, were used to validate the model. Parameter estimates for the velocity, dispersion coefficient, recirculation rate, and the associated 95% confidence intervals were determined by nonlinear least squares regression. Good agreement was shown between the observed tracer breakthrough responses and the simulated concentration history.

NOTATION

A defined in (18).
$\mathbf{b}$ vector of unknown parameters.
B defined in (19).
C liquid phase solute concentration (solute mass/liquid volume), M/L^3.
C_p pulse-injected solute concentration, M/L^3.
C^* solid phase concentration of sorbed solute (solute mass/solids mass), M/M.
D hydrodynamic dispersion coefficient, L^2/t.
$\mathbf{e}$ random vector with zero mean and known covariance matrix.
erfc $[x]$ complementary error function: erfc $[x] = 1 - (2/\sqrt{\pi})\int_0^x e^{-z^2}\,dz$.
$\mathbf{g}$ vector of model simulated data.
G defined in (20).
k, n integers.
K_d partition or distribution coefficient (liquid volume/solids mass), L^3/M.
l location of extraction well, L.
L^{-1} Laplace inverse operator.
m integer summation index.
M, N defined in (8) and (9), respectively.
q fraction of recirculating solute mass: $0 \le g \le 1$.
R retardation factor.
s Laplace transform variable.
S objective function.
t time, t.
t_p duration of the solute pulse, t.
$\mathbf{u}$ vector of independent variables.
U average interstitial velocity, L/t.
x spatial coordinate in the direction of flow, L.
$\mathbf{y}$ vector of observed data.
γ Laplace transform variable.
Γ defined in (21).
θ porosity (liquid volume/aquifer volume), L^3/L^3.
ρ bulk density of the solid matrix (solids mass/aquifer volume), M/L^3.
Φ defined in (22*b*).
Ω defined in (15*b*)

A tilde indicates Laplace transform, and a circumflex represents an estimate.

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