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MASTER

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TRACER TRANSPORT MODELING OF THE DOUBLET WELL SYSTEM

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Steady-state flow and tracer transport between an injection well and a pumping well in a heterogeneous confined aquifer were investigated with numerical modeling. Calculation of transport was based on the advective model for heterogeneous aquifers. Dispersion was assumed to be controlled by microscale velocity variation. An effective parameter of dispersion evaluated on the breakthrough curves was defined to account for the influences of heterogeneity. Breakthrough curves were calculated by using numerical modeling of transport in a strongly heterogeneous aquifer with spatial heterogeneous transmissivity fields. The results of modeling were processed by comparison with analytical solutions of doublet systems to obtain the effective parameters. A special solution was developed for advective transport in aquifers with a layered structure. Examples of real field heterogeneity were given to show its influence on breakthrough curves and the resulting impact on the effective macroscopic parameters.

INTRODUCTION

In the design of optimal groundwater remediation in heterogeneous aquifers, one needs to estimate in situ flow and transport parameters. One effective method for field-scale determination of transport parameters is a tracer test during well injection. There are two common test schemes: the radial flow test during injection in a single well and the horizontal doublet test with a divergent-convergent flow pattern in two wells. The doublet test is considered to be more appropriate for heterogeneous aquifers as indicated by *Mironenko and Rumynin* [1986].

The goal of the present study was to investigate the influences of spatial heterogeneity on breakthrough curves in the pumping well of a doublet system and to calculate the effective transport parameters for such a system.

Radial flow and transport in heterogeneous media have been investigated by several authors, including *Shvidler* [1964], *Desbarats* [1992], *Moreno and Tsang et al.* [1988], *Vandenberg* [1977], and *Mironenko and Rumynin* [1986]. Flow in a multiple-well system in heterogeneous media was studied by *Gomez-Hernandez and Gorelick* [1989], and by *Desbarats* [1993]. Transport problems for such systems using advective and advective dispersive approaches were studied by *Grove* [1971] and *Mironenko and Rumynin* [1986], who obtained analytical solutions for the advective-dispersive problem for the scale of heterogeneity much less than a doublet dimension (the distance between the injection and pumping wells). For a strongly heterogeneous aquifer, it is more common that the difference between the doublet dimension and the heterogeneity scale is not significant.

CURRENT STUDY

The advantages of the horizontal doublet test scheme for the entire thickness of the aquifer have been discussed by *Mironenko and Rumynin* [1986]. Given the same well yield, the flow lines of a doublet form a closed circuit between the wells, thus efficiently averaging the aquifer properties over the doublet's area of influence. It seems that this advantage may be only for the case where the doublet dimension is much longer than the scale of heterogeneity. For many fractured and porous aquifers, however, the horizontal scale of heterogeneity of hydraulic permeability or transmissivity can be tens to hundreds of meters. From a practical point of view, the doublet dimension usually does not exceed two hundred meters because of the long time period required for the test.

The calculation assumes a doublet dimension of 190 m and a heterogeneity scale of 50 m. This is an extreme case as a practical field test, but it still permits analysis of the influence of the realistic field scale heterogeneity. The aim is to determine the effect of transmissivity heterogeneity on the results of the tracer test. The influences of the porosity variation, natural flow gradient, and vertical flow velocity are not considered in this paper.

Aquifer parameters used

The anisotropic exponential model of log transmissivity correlation was chosen for modeling the random aquifer heterogeneity [*Tompson and Gelhar*, 1990]. The variance of log transmissivity was 1.1. That exceeded the number of estimation of the aquifer macrodispersion property within the framework of stochastic hydrology theory [*Gelhar*, 1986]. Modeling the random field of transmissivity with such a large value of variance could lead to abnormally high (on the order of $n \times 10^4$ m²/day) and abnormally low (less than 10^{-3} m²/day) transmissivity values. That is why a limited distribution was sought that would better describe the values near the small and large probability values but give values for the lognormal distribution near the median. The Johnson's S-V distribution, which is normal for the transformed function F_T , was chosen.

$$F_T = \log \frac{T - T_{\min}}{T_{\max} - T} \quad (1)$$

where T is transmissivity and $T_{\min}$ and $T_{\max}$ are its minimum and maximum possible values. The horizontal correlation scales of F_T were $L_x = 30$ m and $L_y = 90$ m. For the random field simulation, the "source point method" of *Ghori et al.* [1993] was used. The transformation used to obtain the random transmissivity field is performed in two steps: (1) Obtain the F_T distribution for the F_T function:

$$F_T(x,y) = M_F + \sigma_F f(x,y) \quad (2)$$

where $F_T(x,y)$ is the F_T function at the point with coordinates x, y ; M_F is the mean value of F_T ; σ_F is the variance; and $f(x,y)$ is a unit random process with the defined autocorrelation function $R(\bar{r})$.

(2) Transform $F_T(x,y)$ into $T(x,y)$ according to

$$T = \frac{T_{\max} \exp(F_T) + T_{\min}}{1 + \exp(F_T)} \quad (3)$$

The parameters of the transmissivity distribution are $M_F = -2.73$, $\sigma_F = 2.0$, $T_{\min} = 0.4$ m²/day, $T_{\max} = 870$ m²/day. The average transmissivity value is 53 m²/day. The aquifer porosity n is assumed to be equal to 0.004. The aquifer thickness m was also constant and equal to 40 m. The microdispersivity parameters were defined as $\lambda_L = 0.05$ m and $\lambda_T = 0.01$ m. The coefficient of molecular diffusion was assumed to be equal to 0. Sorption retardation and tracer decay were neglected.

Doublet test setup

The distance between wells R, was 190 m. The doublet recharge-discharge flow rate Q was chosen to be 300 m³/day. Such a value, given the actual well radius and the interwell spacing of 190 m, yields an average head difference value of 8-15 m, which is quite realistic for the field tests. The tracer injection period was assumed to be 100 days. According to the analytical solution for a homogeneous aquifer, after this period the concentration in the pumping well certainly exceeds 0.5 times the injection concentration.

Simulation of the doublet system was conducted for 25 realizations of a random transmissivity field. For each realization of the field, two tests were simulated:

- (1) the doublet axis lies along the direction of the larger transmissivity correlation scale;
- (2) the doublet axis lies normal to the direction of the larger correlation scale.

NUMERICAL MODELING

To simulate the doublet tests, the numerical code ASM by *Kinzelbach and Rausch* [1991] was used. This code allows simulation of 2D steady or unsteady state flow by the finite difference method and that of contaminant transport by the random walk particle tracing technique [Kinzelbach, 1988, Uffink, 1988]. Displacement of a particle decomposed into the advective component is calculated by the particle tracking technique, and the dispersive component is calculated by random walk at each point.

A strongly divergent or convergent flow on a rectangular grid presents a major problem in modeling. In such cases, as noted by *El-Kadi* [1988], particle tracking can lead to serious errors. To avoid these errors, for interpolation of the nodes nearest to the source or sink, the original ASM code was improved by using a logarithmic rather than linear form. Another source of error in the simulation of a heterogeneous system could be connected with the bilinear velocity interpolation scheme. As has been discussed by *Goode* [1990] the bilinear gradient interpolation scheme would be better for such modeling. After this improvement, numerical modeling with ASM of advective doublet flow for the homogeneous system gave results that when compared with the approximate analytical solution of *Mironenko and Rumynin* [1986], showed good agreement in terms of breakthrough curves.

The size of the model domain was 960 × 960 m, covered by a 60 × 60 grid. Two boundary blocks were defined at each of the four sides with widths of 100 m. The 56 other internal grid steps were constant and equal to 10 m. The doublet axis was parallel to one of the grid directions. The halfway point between wells was at the center of the grid domain. The ratio of

the grid step to the minimum correlation length was 0.3, which, according to a number of studies (Tsang *et al.* [1988], *Tompson and Gelhar* [1990], *Desbarats* [1993]), is quite satisfactory.

The external boundaries were defined as closed and the well's flow rate as constant. Steady hydraulic head and flow velocity fields were obtained by solving the flow equation with the conjugate gradient method. The modeling time step for tracer injection during 100 days was 0.1 day (which is essentially lower than the Courant grid criterion). The number of particles used was 2000. The particles were initially distributed on a circle with a 10 m radius around the injection well.

To monitor the tracer arrival, two observation points were chosen on the doublet axis, one halfway between the wells and the other at 1/4 the distance from the pumping well. Fields for head, velocity, and concentration; breakthrough curves for the pumping well; and observation points were calculated and recorded in the data base after each simulation.

RESULTS

As an example of the simulation results, Fig. 1 shows the fraction of extracted over injected tracer as a function of time for a number of realizations. Averaged breakthrough curves for the pumping well are found in Fig. 2.

The modeling results were processed to estimate the effective porosity value. This was based on the approximate solution for advective transport (*Mironenko and Rumynin* [1986]). This particular solution was chosen as a basis because the solutions (*Grove* [1971], *Mironenko and Rumynin* [1986]) showed little influence of the longitudinal microdispersion over a broad range of Peclet number values.

According to the above solution, the dimensionless concentration C in the pumping well is given by:

$$C(\tau) = \pi^{-1} \inf F(\psi), \quad \tau = \frac{tQ}{\pi R^2 n m}, \quad F(\psi) = \frac{\sin \psi - \psi \cos \psi}{\sin^3 \psi} = \tau \quad (4)$$

where $\inf$ is the function inverse to F . Here, $C = 0$ for time $t < t_0 = 1/3$ and $C > 0$ for $t > t_0$ (Fig. 2) which enables one to use the onset time of tracer arrival (t_0) as an interpretation parameter.

$$n = \frac{3t_0 Q}{\pi R^2 m}. \quad (5)$$

More reliable results could be found, however, by using the information on all breakthrough curves in terms of the extracted dimensionless volume of tracer V .

$$V = \int_{\tau_0}^{\tau} C(\tau) d\tau / (Q \tau_0) = F_v(\tau/\tau_0). \quad (6)$$

From the calculated extracted volume V_f as a function of t , one can use the nonlinear curve fitting method to find the best fit to the $V_f(t/t_0)$ and $V(\tau/\tau_0)$ curves. Then the porosity n can be calculated through the estimated t_0 value.

Both procedures were used for processing the modeling results, which are shown in Table 1.

Table 1

	Doublet axis along the direction of largest correlation scale	Doublet axis normal to the direction of largest correlation scale
Mean value n/n_0 where $n_0 = 0.004$	0.70 0.74	1.04 0.95
Standard deviation	0.26 0.25	0.50 0.17

*The first value is based on the tracer arrival time method, and the second is based on the extracted volume curve fitting method.

Fig. 1. An example of breakthrough curves.

One can find from Table 1 that the difference between results with the arrival time methods and those with the integral method is not significant, but the second method demands a longer testing time.

The modeling confirmed the advantages of doublet tests. Even under such a highly heterogeneous system, the doublet test results show high stability of the calculated parameter for porosity.

Fig. 2. Averaged breakthrough curves.

DISCUSSION

One can see from Fig. 3 that the tracer plume body has a very asymmetrical shape. An analytical solution would give a symmetric picture according to flow lines. Taking into account the changing lengths of flow lines could improve the analytical solution in terms of macrodispersivity. The question is how can one correlate the change of flow paths with the stochastic parameters of the transmissivity field?

A serious question is the influence of the vertical structure of the aquifer on the breakthrough curve. In most porous and fractured aquifers, the permeability and porosity change considerably with depth. To estimate the influence of vertical heterogeneity, a layered transport calculation

scheme could be used. Let us consider an aquifer with thickness m and total transmissivity T to be composed of N layers ($N \rightarrow \infty$) with porosity n_i and hydraulic conductivity k_i . According to this scheme, the Darcy velocity v_i is equal to Q_i/m_i in the i -th interlayer. This is determined as $Q \times k_i/T$. The advective velocity for this layer is equal to v_i/n_i . Changes in advective velocities for various layers, as determined by k_i/n_i , with depth are the reason that pathlines in different layers have different arrival times to the pumping well. For this scheme, let us introduce the time-dependent dimensionless concentration function $C(\tau)$ for an aquifer that is vertically homogeneous with depth. One can then calculate the time-dependent $C(\tau, \chi)$ function according to

$$C(\tau, \chi) = (m^{-1}) \int_0^m C(\tau^* \chi(z)) dz, \quad \chi(z) = \frac{k(z)}{n(z)}. \quad (7)$$

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Fig. 3. A example of the plume body for the time of tracer coming to the pumping well. Injection well is at the point (180, 270) meters. Pumping well is at point 370, 270)

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