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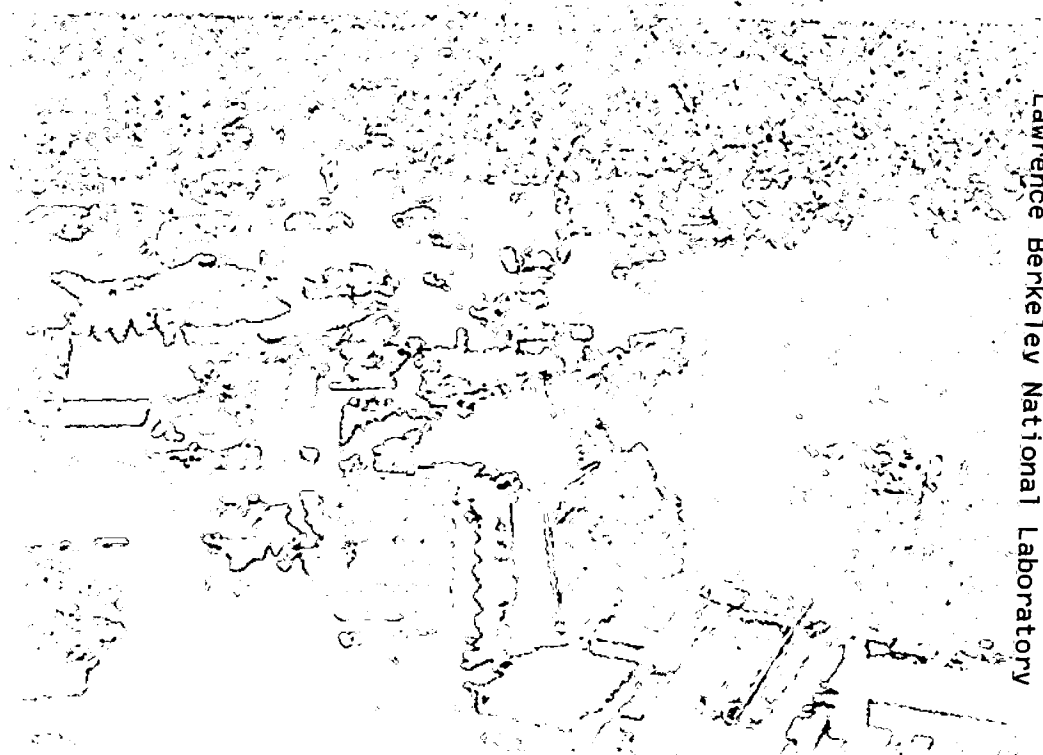
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Earth Sciences Division

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**A Particle-Tracking Method for Advective Transport
in Fractures with Diffusion into Finite Matrix Blocks with
Application to Tracer Injection-Withdrawal Testing**

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ABSTRACT

A particle-tracking method has been developed to calculate tracer transport in fractures with diffusion into finite rock matrix blocks. The method is an extension of the work of Yamashita and Kimura (1990), which is only applicable to diffusion into an infinite matrix. The new method has been verified against a number of analytic or semi-analytic solutions for transport in a homogeneous fracture medium with matrix diffusion. The method is applied to the calculation of tracer breakthrough curves for a hypothetical tracer injection-withdrawal experiment in a heterogeneous fracture zone, with variable hydraulic properties and finite matrix blocks.

INTRODUCTION

The importance of matrix diffusion and sorption for the transport of tracers in fractured porous rocks is well recognized [Neretnieks, 1980]. A number of methods have been developed for the calculation of these processes [e.g., Tang *et al.*, 1981; Rasmuson and Neretnieks, 1981; Barker, 1982, 1985; Sudicky and Frind, 1982; Maloszewski and Zuber, 1990, 1993; Quinodoz and Valocchi, 1993; Moench, 1995; and Cvetkovic *et al.*, 1999]. This paper presents a particle-tracking technique to calculate the effects of matrix diffusion and sorption on tracer transport and breakthrough curves. The technique is based on a procedure proposed by Yamashita and Kimura [1990] for calculation of diffusion into an infinite matrix medium. However, an infinite matrix is not realistic, as in practice one encounters diffusion into matrix blocks or layers of finite dimensions. In this paper, we have extended the particle tracking technique to the case of finite matrix blocks, and to the case involving heterogeneous systems, both of which cannot be easily handled by conventional methods. The proposed technique can be applied easily to a complex heterogeneous fracture system within the framework of a discrete fracture network or of a dual-porosity model, so long as a flow field is first calculated.

THEORY AND PROCEDURE

Let us assume that we have a steady-state flow field, which may have been calculated, for instance, by applying finite-difference or finite-element methods to a heterogeneous fracture continuum. The particle-tracking method involves the release at source locations of a large number of particles representing solutes, or tracers, and these are followed step by step as they move from grid cell to grid cell. Following chemical engineering practice, the residence time t_w (without matrix diffusion) during which a particle resides within a grid cell without a source or sink is given by:

$$t_w = \frac{\phi_f \Delta x \Delta y \Delta z}{\frac{1}{2} \sum_j |Q_{ij}|} \quad (1)$$

where Δx , Δy , Δz are the dimensions of the grid cell i , ϕ_f is the fracture porosity of the medium, and Q_{ij} is the flow rate in volume per time between the cell of interest, i , and its neighbors j . After this residence time, outgoing tracer particles are distributed to the neighboring grid cells according to stream tubes, given that Q_{ij} (for all j) is known [Moreno *et al.*, 1990].

The effect of diffusion and linear sorption is represented by an increase in the particle residence time from t_w to a new time interval, t . In order to calculate the increased residence time, we use a solution for the tracer concentration attenuation over time, assuming the flow to be in contact with the matrix block into which diffusion occurs. The ratio of the concentration C exiting the grid cell over the initial concentration C_0 entering the grid cell may be written as:

$$C/C_0 = f(t, t_w, m_1, m_2, \dots) \quad (2)$$

The left hand side varies from 0 to 1, and is dependent on t_w , the tracer residence time in the absence of matrix diffusion, and the other parameters $m_1, m_2, \dots$ which specify properties of the rock matrix, such as porosity, matrix diffusion and sorption coefficients. To incorporate the effects of matrix diffusion into particle tracking, we follow the procedure of Yamashita and Kimura [1990], who proposed the use of a number R drawn randomly from the uniform distribution $U[0,1]$ and equated with C/C_0 . Then, the residence time t for each particle in a discretized element, incorporating the effect of diffusion, is inversely calculated from the equation:

$$R=f(t, t_w, m_1, m_2, \dots), \quad (3)$$

where all variables other than t (i.e., $t_w, m_1, m_2, \dots$) are known.

At this point, the particle residence time for the grid cell t_w is replaced by t , the increased residence time as a result of the diffusion of the particle into the matrix. As a large number of particles traverse the field in this manner, they are collected at observation points, such as a pumping well, as a function of their cumulative travel times since release at the source. The result is a tracer breakthrough curve. Assuming all the particles were released at the same time, the breakthrough curve will correspond to a tracer pulse injection. Generally if we define appropriately the particle release times at the source, we can calculate the breakthrough curves for any given tracer injection with variable concentration. For the remainder of the paper we shall consider only the case of tracer injection with a single concentration pulse at time 0.

To study the effect of diffusion into finite matrix blocks, we select from the literature, somewhat arbitrarily, the solution of *Rasmusson and Neretnieks* [1981] for the function $f(t, t_w, m, m_2, \dots)$ in Equation (3). In their model, the tracer flows in orthogonal sets of fractures forming a regular network in 3-D, and the matrix volume between fractures are represented by spherical matrix blocks of radius r_m . Thus, the fracture-to-fracture spacing is $\lambda=2r_m$. The solution is given in terms of an infinite integral. A special case for a non-sorbing tracer with negligible longitudinal dispersion (i.e., Peclet number $Pe \rightarrow \infty$) is used for our calculations. The solution in this case can be written as:

$$\frac{C}{C_o} = \frac{1}{2} + \frac{2}{\pi} \int_0^{\infty} \exp(-\delta_o H_1) \sin(y \omega^2 - \delta_o H_2) \frac{d\omega}{\omega} \quad (4)$$

where

$$y = 2 \frac{D_e}{\phi_m r_m^2} (t - t_w)$$

$$\delta_o = 3 \frac{D_e}{r_m^2} \frac{(1 - \phi_f)}{\phi_f} t_w$$

$$H_1(\omega) = \omega \left(\frac{\sinh 2\omega + \sin 2\omega}{\cosh 2\omega - \cos 2\omega} \right) - 1$$

$$H_2(\omega) = \omega \left(\frac{\sinh 2\omega - \sin 2\omega}{\cosh 2\omega - \cos 2\omega} \right)$$

and ϕ_m , matrix porosity; ϕ_f , fracture porosity; D_e , effective diffusion coefficient in the matrix pores (L^2/T), which is equal to $D \cdot \tau \cdot \phi_m$; τ , tortuosity (< 1); D , free water diffusion coefficient (L^2/T); and ω , the integration variable.

The fracture porosity ϕ_f is related to the fracture aperture b by:

$$m (b / \lambda) = \phi_f \quad (5)$$

where λ is the fracture spacing, and $m = 1$ corresponds to the case where the fractures are parallel and non-intersecting, and $m = 3$ corresponds to the case where the fractures form three orthogonal and intersecting sets. The fracture spacing λ can also be thought of as the matrix block length.

Our definition of D_e differs from that of *Tang et al.* [1981] by the factor of ϕ_m (Tang's effective diffusion coefficient is the product of only D and τ). The parameter groups denoted by y and δ_o have, respectively, the physical meaning of a dimensionless increased residence time produced by diffusion into finite matrix blocks, and the ratio of

the advective time t_w to the diffusion time into the matrix blocks. Thus, Equation (4) describes the concentration of the particles which, moving in a fracture continuum with a given fracture porosity ϕ_f , are allowed also to diffuse into finite matrix blocks with radius r_m , porosity ϕ_m , and tortuosity τ .

So, given a generated random value R for C/C_0 , y in Equation (4), and ultimately t , can be evaluated for a range of δ_0 values. This is done by interpolation from a table of calculated sets of $(\delta_0, C/C_0, y)$ values. The interpolation works well if the set of three numbers are densely and evenly spaced in the parameter space of C/C_0 and δ_0 . After some experimentation, we found that this can be facilitated by evaluating C/C_0 versus y/δ_0 for $\delta_0 > 1$, and C/C_0 versus y/δ_0^2 for $\delta_0 < 1$.

The interpolation method can be described by reference to Figure 1. Given the parameter values for the flow system and t_w , δ_0 can be calculated. Then, the appropriate curve for the specific δ_0 value is chosen and the corresponding value on the horizontal axis for a particular $R=C/C_0$ value is found. This value is equal to y/δ_0 if $\delta_0 > 1$ or y/δ_0^2 if $\delta_0 < 1$. The diffusion-increased residence time t is then readily computed from this value.

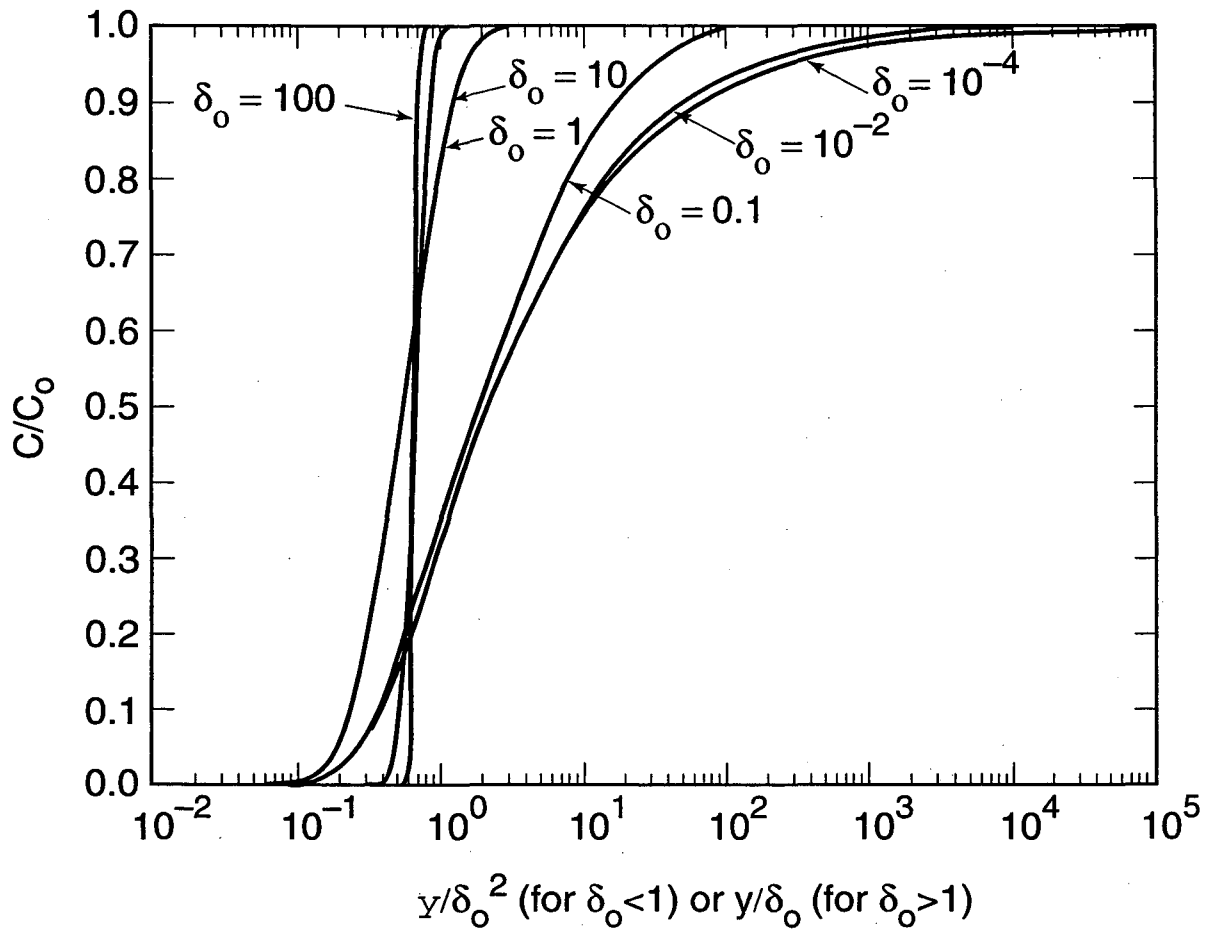


Figure 1. Relationship between C/C_0 , δ_0 , and y . The x-axis is plotted as y/δ_0^2 and y/δ_0 depending on whether δ_0 is smaller or larger than 1, respectively.

Equation (4) describes diffusion into finite rock matrix blocks. For diffusion into an infinite matrix, a simpler solution is available. Consider a parallel-plate fracture of constant aperture (b), and width (w), imbedded in an infinite matrix medium. For one-dimensional steady-state flow rate Q , the advective residence time for plug flow without matrix diffusion over a distance of L in the fracture is $t_w = Lwb/Q$. Assuming diffusion into an infinite matrix medium in the direction normal to the advective flow direction, an analytical solution [Neretnieks, 1980] is available:

$$\frac{C}{C_o} = \text{erfc} \left(\frac{(k_d \rho_p D_e)^{1/2} t_w}{(t - t_w)^{1/2} b} \right) \quad (6)$$

where D_e is the effective diffusion coefficient in the matrix pores (L^2/T); k_d is the linear sorption coefficient (L^3/M) and ρ_p is the rock matrix density (M/L^3). For a non-sorbing tracer, $k_d \rho_p$ is simply the matrix porosity ϕ_m .

Equation (6) is shown in Figure 2 for different values of the parameter group,

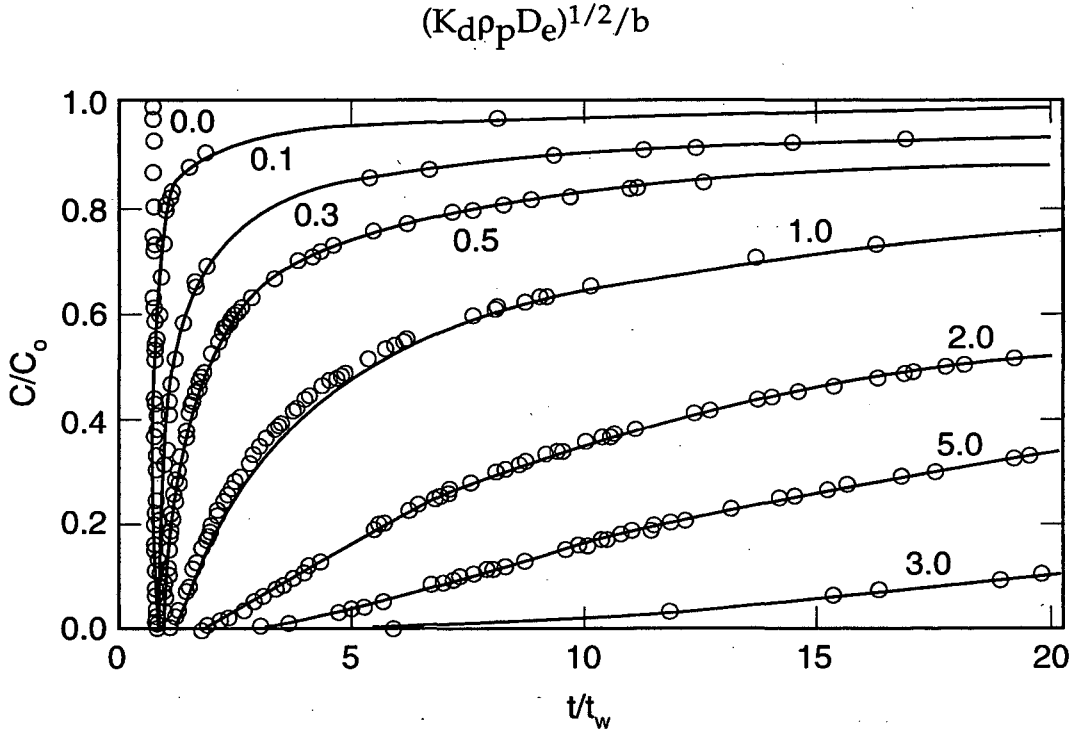


Figure 2. Forward and inverse calculations (lines and circles respectively) of the particle residence times based on Equation (5), with different values of the parameter group $(K_d \rho_p D_e)^{1/2} / b$, which label the curves.

In terms of our particle tracking method, the implementation of Equation (6) is much simpler than that for Equation (4). Here, once the system parameters are specified, Equation (6) can be used directly to compute t/t_w from $R = C/C_o$, corresponding to one particular curve in Figure 2. This is unlike Equation (4) where interpolation using a set of

curves is required (Figure 1), since calculation of t/t_w depends not only on system parameters but also on t_w . Computationally, particle tracking based on Equation (6) is a factor of three to four more efficient than that based on Equation (4).

Particle tracking calculations based on Equations (4) and (6) should give the same results when the penetration of the tracer into the matrix is negligible compared with the matrix block size. Therefore a criterion for the use of the simpler and computationally more efficient Equation (6) may be developed as follows. The concentration in the matrix as a function of penetration depth from the fracture-matrix interface can be written as (*Carslaw and Jaeger*, 1959: p.60, Eq. 10):

$$\frac{C}{C_o} = \text{erfc} \frac{z}{2(D_e t)^{1/2}} \quad (7)$$

Let us assume that the impact of finite block size is negligible if the concentration at the center of the matrix block is small, specifically if $C/C_o < 0.01$. Setting the right side of Equation (7) to be less than 0.01, we calculate that the argument for the complementary error function should be greater than 1.82, or 2 by rounding-off to integer. By setting $z = r_m$, the early time criterion for Equation (6) to be valid becomes $t < r_m^2/16D_e$.

A code named THEMM (Transport in Heterogeneous Medium with Matrix Diffusion) was developed to calculate flow in a general heterogeneous permeability field, with the finite difference technique and transport with the particle tracking method described above. This code allows the user to choose either Equation (4) or Equation (6) for the diffusion calculation.

VERIFICATION OF THE TECHNIQUE

The proposed particle-tracking method was verified against three analytical or semi-analytical solutions for transport in homogeneous media [Tang et al. (1981), Chen (1986) and Moench (1995)]. Unfortunately no such solutions are available for heterogeneous fields, for which the particle-tracking method has been designed.

Verification Problem 1: Linear Flow

Tang et al. [1981] provides an analytical solution for tracer concentration as a function of distance and transport time for 1-D linear flow in a single fracture, with matrix diffusion into the infinite rock matrix.

$$\frac{C}{C_o} = \operatorname{erfc} \left[\frac{z\phi_m\sqrt{D\tau}}{v^{1/2}(vt-z)^{1/2}\delta} \right] \quad (8)$$

The symbols are explained in Table 1, together with the numerical values used in the verification exercise.

Note that Equation (8) is essentially the same as Equation (6). It assumes infinite matrix blocks, which is valid for a time period satisfying the early time criterion. If we assume that $r_m = 1.5$ m, a choice of time $t = 10^5$ s will certainly satisfy the condition. For verification purpose, the THEM code is used with both finite and infinite block solutions - Equations (4) and (5). Figure 3 shows the comparison. The agreement is very good between the analytic solutions and our particle-tracking method. As to be expected, the particle tracking results from Equations (4) and (6) are essentially the same.

Table 1. Parameters and Values used in the Three Verification Examples.

Verification Problem 1: Linear Flow		
v	velocity	10^{-4} m/s
b	fracture aperture	10^{-3} m
D	free water diffusion	7.4×10^{-10} m ² /s
τ	tortuosity	0.11
ϕ_m	matrix porosity	0.16
Verification Problem 2: Radial Divergent Flow		
Q	injection rate	1.157×10^{-7} m ³ /s
r_w	wellbore radius	0.11 m
b	fracture aperture	10^{-4} m
α	longitudinal dispersivity	0.5 m
D	free water diffusion coefficient	1.6×10^{-9} m ² /s
τ	tortuosity	0.1
ϕ_f	fracture porosity	10^{-4}
ϕ_m	matrix porosity	0.01
Verification Problem 3: Radial Convergent Flow; Finite Matrix Block		
Q	pumping rate	1.0×10^{-3} m ³ /s
h	aquifer thickness	7.0 m
r_w	pumped well radius	0.4 m
r_L	distance of injection to pumped well	20 m
D	free water diffusion coefficient	7.2×10^{-10} m ² /s
τ	tortuosity	0.1
ϕ_f	fracture porosity	0.0015
ϕ_m	matrix porosity	0.15
$2r_m$	fracture spacing ($\gamma = 10^{-5}$, 10^{-3} , 10^{-1} , 10 respectively)	6.158m, 0.6158m, 0.06158m, 0.006158m)

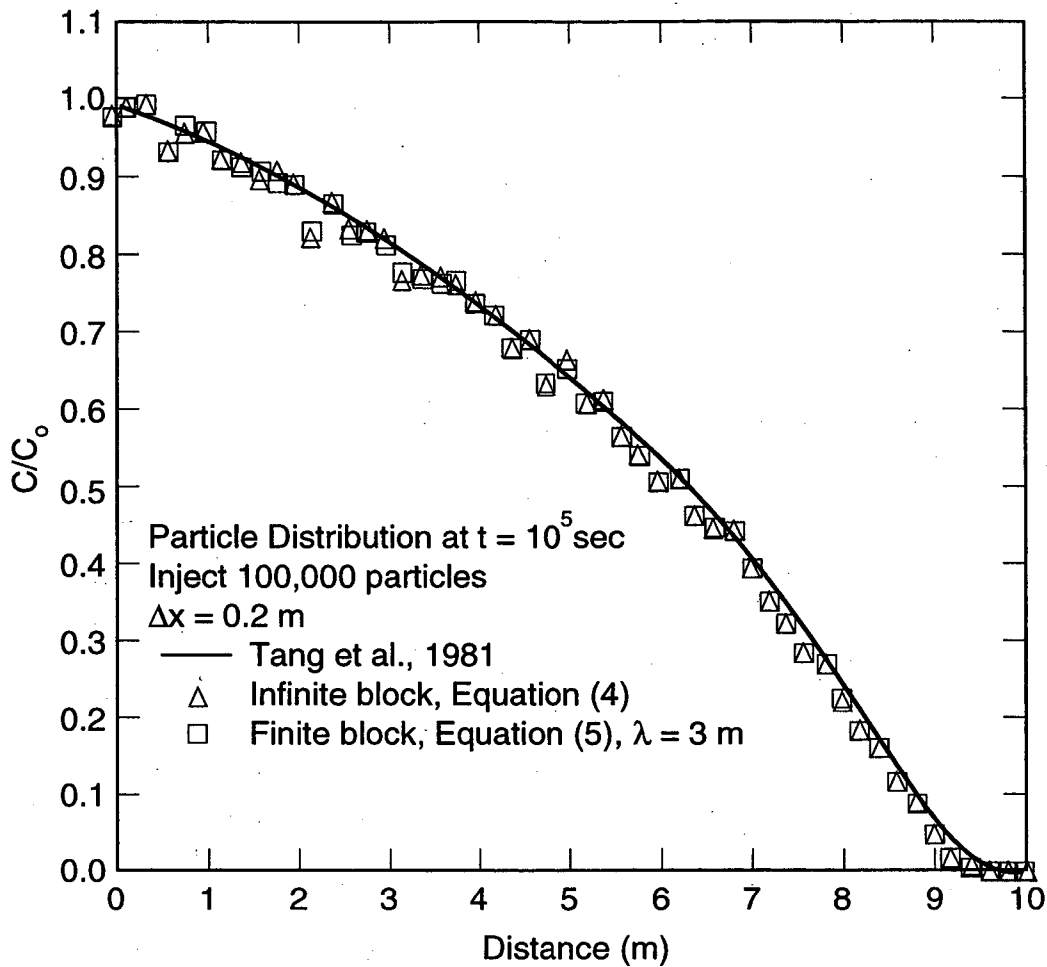


Figure 3. Comparison of THEMM results with the analytical solution of Tang et al. (1981). Tracer concentration is shown as a function of linear distance from the injection well.

Verification Problem 2: Radial Divergent Flow

An analytic solution for radially divergent, steady flow and transport in a fracture with diffusion into infinite matrix is given by Chen [1986]. He considered two models: Model I, which includes radial advection and longitudinal dispersion in the fracture plane, and Model II, which includes radial advection only. He also considered two boundary conditions at the tracer source, namely, constant concentration condition or a decaying-concentration condition. The solution of Model I is given in the Laplace

domain in terms of Airy functions and is evaluated by numerical inversion of the Laplace transforms. Small-time and long-time approximate solutions (which will not be reproduced here) are also derived by Chen [1986].

The solution for Model II is given by Chen [1986] in terms of complementary error function. For verification of our particle-tracking method, we use zero longitudinal dispersion and constant tracer concentration at the well with radius r_w , where the tracer is injected at a constant rate Q . Under these conditions, Chen's solution [Equation 59 of Chen (1986)] reduces simply to:

$$\frac{C}{C_o} = \text{erfc} \left(\frac{\phi_m \sqrt{D\tau} \pi (r^2 - r_w^2) / Q}{(t - \pi [r^2 - r_w^2] b / Q)} \right) \quad (9)$$

$$\text{for } t < \pi (r^2 - r_w^2) b / Q$$

$$\frac{C}{C_o} = 0 \quad \text{for } t > \pi (r^2 - r_w^2) b / Q$$

The symbols in Equation (9) and their numerical values in the verification exercise are given in Table 1.

Note that Chen [1986] defines the fracture aperture to be $2b$, but we define it as b , so that there is a factor-of-2 difference in the two b values. With this correction, the set of parameters indicated above is exactly the same as those of Chen [1986] in generating Figure 6b of his paper. In the list of parameters, we have included the longitudinal dispersion of 0.5 m. This parameter is not needed for Model II; however, in the results

below we also present, for comparison, Chen's results for Model I, where longitudinal dispersion is included.

Calculations were made for C/C_0 versus r at times 0.01 year, 0.1 year, and 1 year, with increasing radial transport distances. For the particle-tracking calculations using the THEMM code, we have chosen the radial grid lengths of 0.2, 0.5 and 2 m, to calculate results at 0.01, 0.1 and 1 year respectively, so that the accuracies of calculations are approximately the same. For each case, over 100,000 particles are used in the computation. In Figure 4, results of the THEMM code are compared with the results of Chen [1986], taken from Figure 6b of his paper. Excellent agreement can be seen between THEMM and Model II. The Model I results are shown only for comparison purposes to indicate the effects of longitudinal dispersion. Note that for later times, Model II results approach those of Model I, showing that the effect of longitudinal dispersion in the fracture decreases in importance for late-time results.

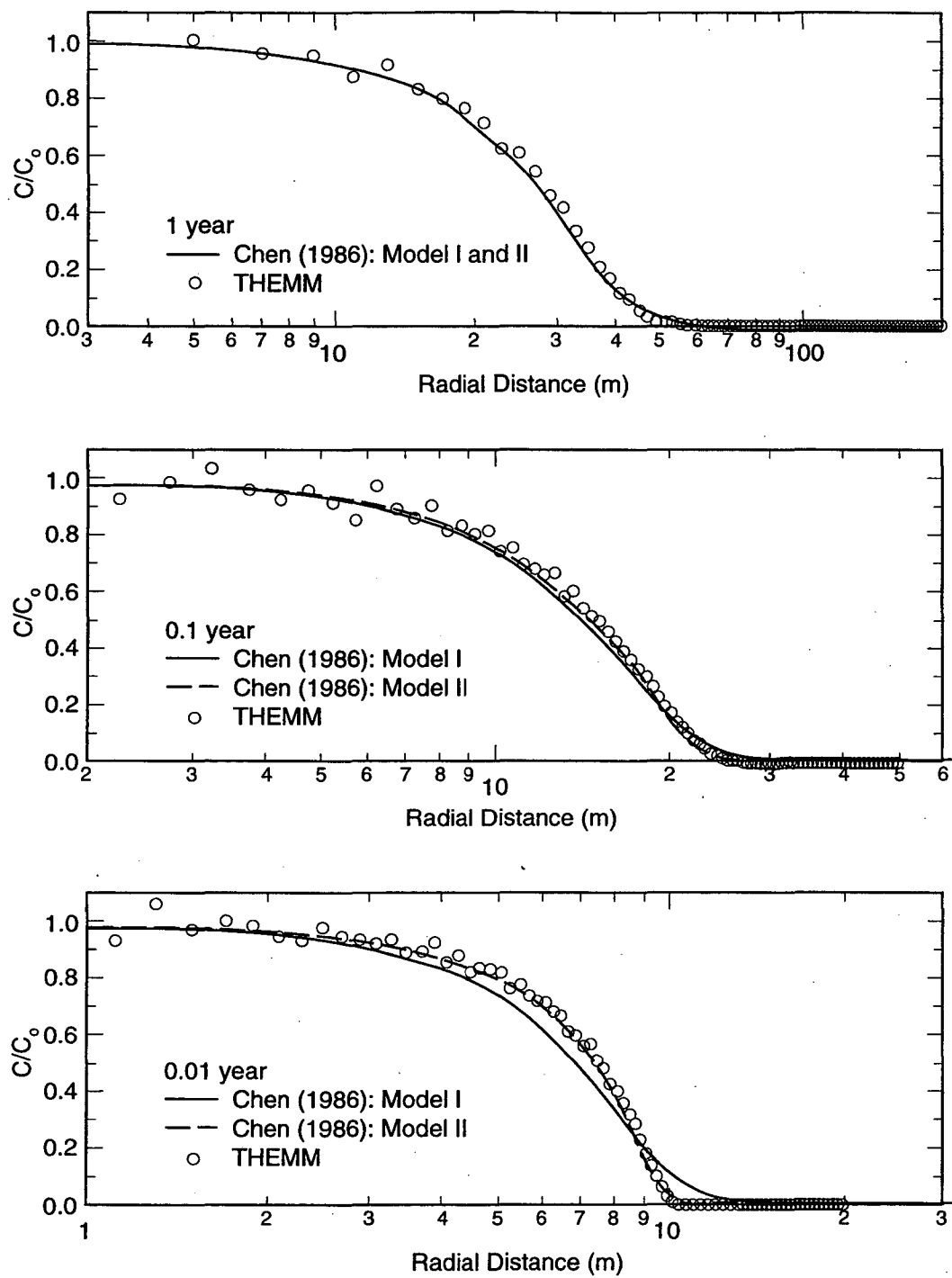


Figure 4. Comparison of THEMM results with the semi-analytic results of Chen (1986). Distribution of tracer concentration is shown as a function of radial distance from the injection well at three injection times as indicated.

Verification Problem 3: Radial Convergent Flow, Finite Matrix Blocks in a Double-Porosity Model

An exact Laplace transform solution was obtained by *Moench* [1995] for the problem of dispersion, advection, and adsorption of a tracer injected into a steady, horizontal, radially convergent flow field in a densely fractured porous formation. The medium is represented by a double-porosity medium with finite matrix blocks. Assuming that the tracer is released at distance r_L from a pumping well, no chemical retardation in the fracture or rock matrix, and no fracture skin effects, the three parameters used by *Moench* [1995] may be defined using our notation as:

$$\begin{aligned} Pe &= r_L / \alpha_L \\ \sigma &= \phi_m \left(\frac{1 - \phi_f}{\phi_f} \right) \\ \gamma &= \frac{D_e}{r_m^2} \frac{(r_L^2 - r_w^2) \pi h \phi_f}{Q} \left(\frac{1 - \phi_f}{\phi_f} \right) \end{aligned} \quad (10)$$

where, in addition to the symbols previously defined, α_L is the longitudinal dispersivity in the fracture, and h is the thickness of the fractured aquifer. Thus, Pe is an inverse measure of the dispersion in the fracture, and σ may be considered as a measure of the double porosity character of the aquifer, so that $\sigma=0$ implies a single-porosity medium with zero matrix diffusion, and $\sigma=100$ implies a double-porosity medium with $\phi_m/\phi_f \sim 100$. The parameter γ is proportional to D_e/r_m^2 and is a measure of diffusion into finite matrix blocks.

Moench's dual-porosity conceptual model corresponds with our formulation of Equation (4) where the 3-D network of fractures are separated by spherical matrix blocks

of radius r_m . Tracer breakthrough curves are calculated using our particle-tracking code THEMM for the case of a pumping well with a constant-concentration tracer source at a distance r_L . Parameter values are taken from *Moench* [1995] and are listed in Table 1. Note that we assume $D_e = D \cdot \tau \cdot \phi_m$ for this comparison. Given the values of ϕ_f and ϕ_m , $\sigma = 100$, corresponding to the set of curves in Figure 3a of *Moench* [1995].

The γ values used in the verification exercise extend over six orders of magnitude, thus covering scenarios ranging from very little diffusion into the matrix to such a large amount of diffusion that the matrix blocks are saturated with tracers and no further diffusion is possible. Figure 5 shows that the breakthrough curves display a piston shape for both small and large values of γ . The difference in time between the various cases is a reflection of the impact of diffusion on the tracer transport.

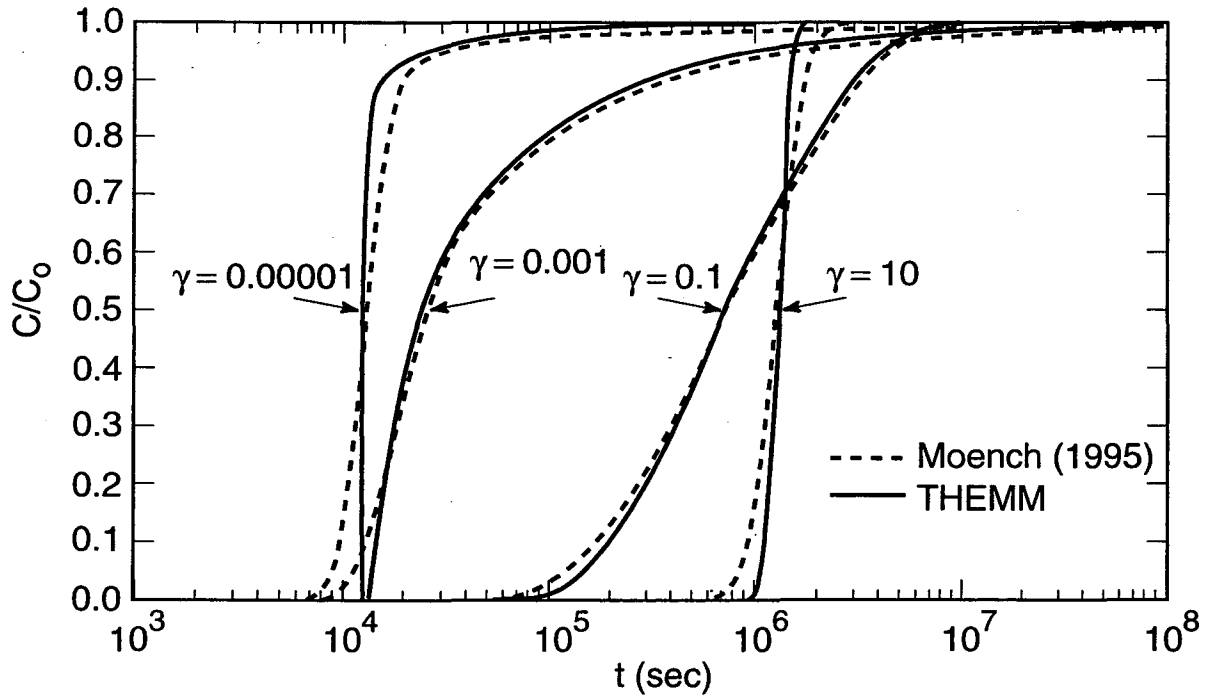


Figure 5. Comparison of THEMM results with the semi-analytical solution of Moench (1995). Tracer concentration at the pumping well is shown as a function of time for different γ values.

The comparison between our particle tracking approach and the solution of Moench is shown in Figure 5. The particle tracking method does not include longitudinal dispersion, whereas Figure 3a of *Moench* [1995] assumes $Pe = 50$, which translates to a dispersivity of 0.4 m. Thus, some difference between the Moench model and the THEMM code is to be expected. Taking this into account, we consider the agreement to be very good.

APPLICATION TO A HYPOTHETICAL INJECTION-WITHDRAWAL EXPERIMENT IN A HETEROGENEOUS MEDIUM

As a non-trivial example demonstrating the capability of the particle tracking technique, let us consider a hypothetical tracer injection-withdrawal test in a single well in a heterogeneous fracture zone (i.e. with spatially varying fracture permeability). This is also sometimes called a “huff-puff” or a “push-pull” test. A tracer is injected for a certain time period and then withdrawn from the same well for an extended time period until almost all the tracer is recovered. One advantage of the injection-withdrawal test is that flow channeling effects produced by permeability heterogeneity [*Moreno and Tsang*, 1994] are cancelled in the injection and withdrawal sequence, since the fast outgoing paths during injection are also the fast incoming paths during withdrawal. Therefore, the diffusive-dispersive phenomenon can be isolated and clearly evaluated. To solve this problem for a heterogeneous fracture permeability field with finite matrix regions between adjacent fractures is a major challenge for conventional approaches. The particle tracking method described in this paper can address it quite efficiently as shown below.

We consider two hypothetical 2-D fractured aquifers: a homogeneous one and one with heterogeneous permeability field generated with the turning bands method

[Tompson et al., 1989]. The heterogeneous field is generated using a standard deviation in natural log permeability (m^2) arbitrarily set to 1.73. In our hypothetical problem, the tracer is first injected at a constant rate for 24 hours. At the end of the first 100 minutes, the front of tracer plumes in the two cases are shown in Figure 6. These tracer fronts are actually the calculated positions of a larger number of particles 100 minutes after they are released at the injection well. Here, one sees that the tracer front is circular for the homogeneous case (as one would expect) and star-shaped for the heterogeneous case.

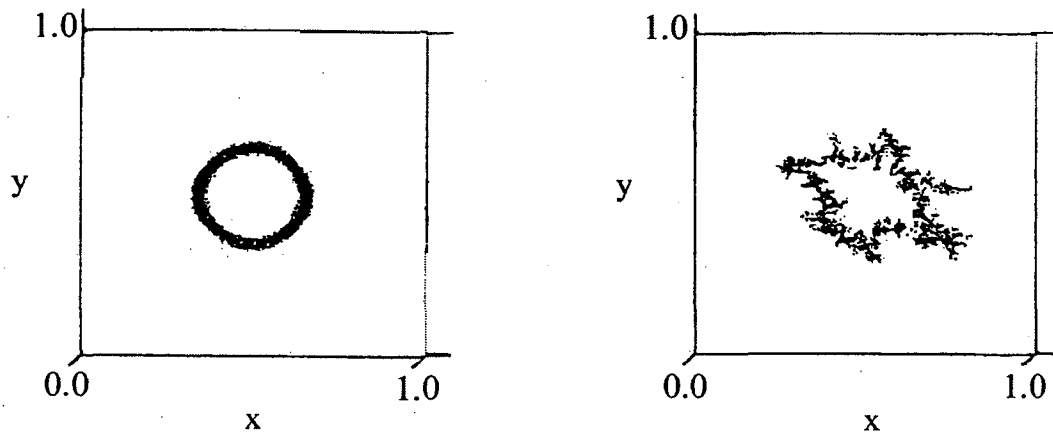


Figure 6. The front of tracer plumes after 100 minutes of injection. The injection well is at (0.5, 0.5). The case for the homogeneous fracture medium is shown on the left and that for the heterogeneous medium is shown on the right.

After 24 hours of tracer injection, the well is switched immediately over to pumping. The tracer production after this switch is calculated with our particle-tracking code THEMME and plotted as cumulative mass recovered over the total injected mass as a function of time. Both the finite matrix case (Equation 4) and the infinite matrix case (Equation 6) are calculated. For the finite block case, the radius of the matrix blocks is assumed to be 5 cm.

The simulation results are shown in Figure 7. The homogeneous and heterogeneous results are almost identical, confirming the hypothesis that test results are not sensitive to the flow channeling produced by heterogeneity. At early times, the finite and infinite block results are similar, but they diverge at later times. For the finite block case, tracer concentration buildup in the matrix during the injection period is much faster, resulting in a strong diffusion back into the fracture during the withdrawal period. In this case, full recovery is found after about 8 months (2×10^7 seconds) of pumping. For the infinite matrix case, the recovery is below 90% even after 10 years (3.2×10^8 seconds).

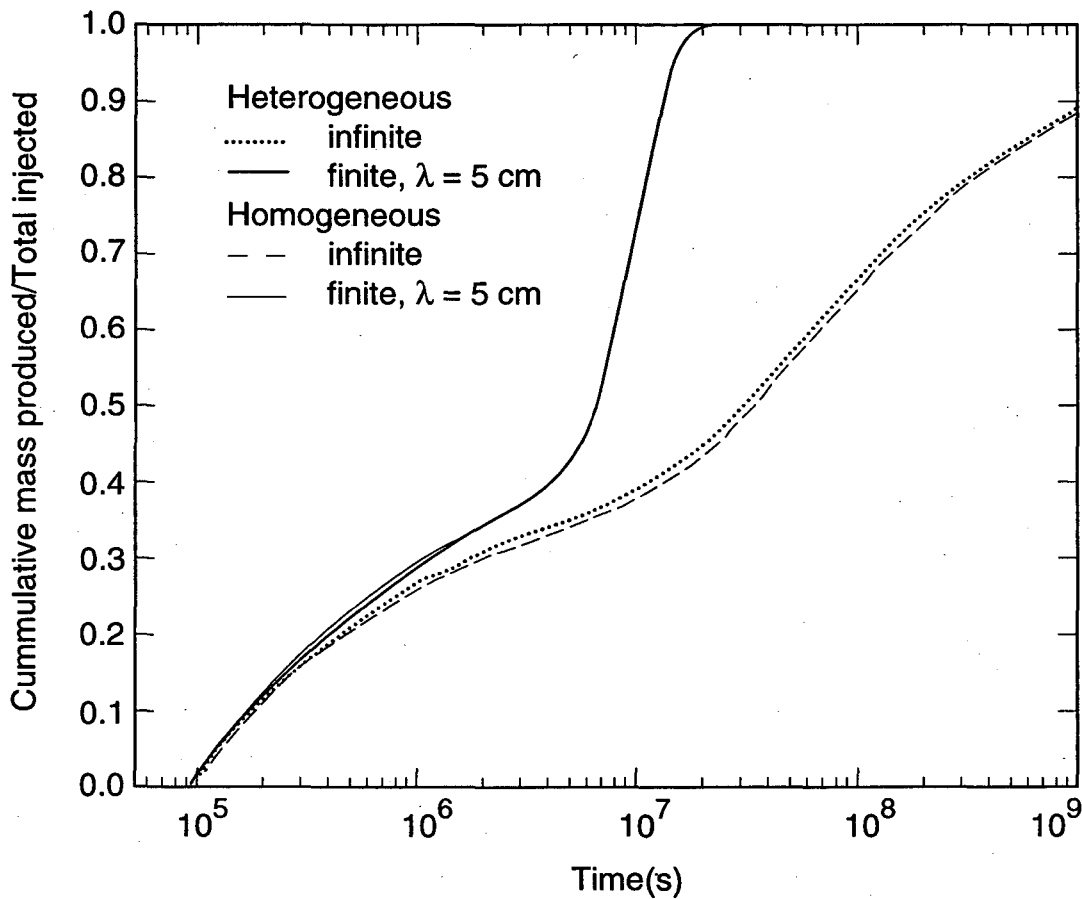


Figure 7. Tracer concentration as cumulative mass recovered divided by the total injected mass as a function of time during the withdrawal period in an injection-withdrawal test.

It is also interesting to note that all the curves in Figure 7 display a two-plateau structure. The first plateau is at $y \sim 0.4$ and the second is at $y = 1.0$. The first plateau represents the tracer mass in the fracture at the time of the switch from injection to withdrawal. The late-time part of the tracer withdrawal curve is controlled by the slower process of tracer diffusion from the matrix into the fracture. The time to recover the tracer from the matrix is several orders of magnitude smaller for the finite-block case than for the infinite-block case, as would be expected.

These numerical simulations may be used to analyze actual *in situ* injection-withdrawal tracer tests and to evaluate the parameters controlling matrix diffusion. This example illustrates the power of our particle tracking method to account for diffusion into finite rock matrix blocks, even in the case of heterogeneous fracture flow fields.

SUMMARY

This paper presents a new particle-tracking technique to calculate diffusion into finite matrix blocks for transport in a heterogeneous fracture system. It can be applied to either a fracture-network model or a dual-porosity model. Results are in good agreement with existing analytic or semi-analytic solutions. An example application of the method to calculate tracer breakthrough curves from a hypothetical tracer injection-withdrawal experiment in a heterogeneous fracture zone with finite matrix blocks demonstrates the utility of this new approach.

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