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**Authors**

Pan, Lehua
Seol, Yongkoo
Bodvarsson, Gudmundur S.

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# Improved estimation of the activity range of particles:
# The influence of water flow through fracture-matrix interface

*Lehua Pan, Yongkoo Seol and Gudmundur S. Bodvarsson*

*Earth Sciences Division, Lawrence Berkeley National Laboratory,Berkeley, CA 94720, USA*

**Abstract**

In our previous paper (Pan and Bodvarsson, 2002), the concept of activity range of particles was introduced within the framework of the dual-continuum random-walk particle tracking approach. This enhanced particle tracking method was shown, through comparison to analytical solutions, to accurately simulate transport within the fracture-matrix system. This method is attractive because it can achieve high accuracy in simulating mass transfer through the fracture-matrix interface without using additional matrix grid-cells (thus maintaining optimum efficiency) and without requiring a passive matrix (thus being applicable to cases where global water flow exists in both continua). Although included in the scheme, the effect of water flow through the fracture-matrix interface (f-m water flow) on the activity range had not yet been tested, because the test cases, for which analytical solutions exist, do not have both f-m water flow and global flow within the matrix. However, for transport in the variably saturated fractured porous media, both f-m water flow and global matrix flow could be significant. The objectives of this study are (1) to investigate the influence of the fracture-matrix water flow on the activity range and (2) to develop improved schemes for calculating the activity range. The improved particle-tracking model will be verified against analytical solutions and a multiple-continuum numerical model (MINC).

The approach proposed by Pan and Bodvarsson (2002) was based on the fact that the penetration of particles are confined within a certain range in the matrix, depending on the time elapsed since the pulse of particles was injected. Such a range is its activity range, which is a function of the particle's "age", $t_p$. Therefore, two key parameters, the characteristic distance $S_{fm}$ and the matrix volume $V_m$, should be replaced (in calculating the particle transfer probability in the dual-continuum particle tracking method) with the effective characteristic distance $S_{fm}(t_p)$ and the effective matrix volume $V_m(t_p)$, respectively. These parameters are related to the activity range in the following manner:

$$S_{fm}(t_p) = S_{fm}\,\frac{B^*(t_p)}{B} \tag{1a}$$

$$V_m(t_p) = V_m\,\frac{B^*(t_p)}{B} \tag{1b}$$

where $B^*(t_p)$ is the activity range, the value of which varies from 0 to B, the maximum activity range (e.g., one-half the fracture spacing for a system of parallel-plate fractures separated by porous rock). Based on the analytical solutions of the one-dimensional diffusion process, Pan and Bodvarsson (2002) found that the activity range is proportional to the square root of $t_p$ if no water flow through the fracture-matrix interface occurs:

$$B^*(t_p) = \min\left(\alpha\sqrt{4\,D_m\,t_p/R_m}\ W(t_p),\ B\right) \tag{2}$$

where the weighting function $W(t_p)$ in (2) was used to account for the secondary effects of the neighboring fractures on the expansion of the activity range. The parameters $\alpha$, $D_m$, and $R_m$ are the empirical coefficient, the effective matrix diffusion coefficient, and the retardation factor in the matrix, respectively. The effect that water flow through the fracture-matrix interface has on the activity range was simply accounted for by assuming a constant velocity from the fracture-matrix interface into the rock matrix (Pan and Bodvarsson, 2002). As a result, the final formula for calculating the activity range was defined as follows:

$$B^*(t_p) = \min\left(\alpha\sqrt{4\,D_m\,t_p/R_m}\ W(t_p) + \text{sign}(q_{fm})\min\left(\frac{|q_{fm}|\,t_p}{\theta_m},\ 2b\right),\ B\right) \tag{3}$$

where 2b is the effective fracture aperture, $\theta_m$ is the volumetric water content in the matrix, and $q_{fm}$ is the water flux at the interface. Equation (3) implies that the activity range $B^*$ as a function of $t_p$ is a simple sum of two components, the diffusion term and the advection term. However, this may not be correct, for the following reasons: (1) the water velocity is not constant away from the fracture-matrix interface (e.g., it becomes zero at the middle point between two parallel fracture planes); and (2) the f-m water flow will interact with the global matrix water flow. As a result, the expansion of the activity range could be very complex if significant f-m water flow exists. Rigorously deriving such a relationship is actually beyond the capabilities of the dual-continuum approach for modeling transport in fractured porous media. This is why Equation (3) limits the influence of the f-m water flow within the confined range of 2b.

Fortunately, the purpose of calculating the activity range is not to describe the details of particle distribution within the matrix block. Instead, it is used to improve the accuracy of calculating the particle transfer probability of particles between the fractures and the matrix. Furthermore, in the dual-continuum model, the fracture-matrix connection actually constitutes the fourth dimension of a 4-D space. Therefore, we can focus on the first problem mentioned above (varying water velocity away from the f-m interface). Because there is no closed-form analytical solution available for the cases with variable water flux, we start with the previously used analytical solution with constant water flux (Pan and Bodvarsson, 2002) and take it as a good approximation. A new cross-interaction term is introduced to account for the effects of the varying f-m water flow on the activity range. As a result, we propose the following schemes to calculate the activity range:

$$B^*(t_p) = \min\left(\sqrt{\left(\alpha^2 + \frac{q_{fm}t_p}{\theta_m B}\right)4\,D_m\,t_p/R_m}\ W(t_p) + \frac{q_{fm}\,t_p}{\theta_m},\ B\right) \tag{4}$$

This new scheme (4) includes a term that represents the influence of the f-m water flow on the f-m diffusion process. Quantitatively, the term $(-q_{fm}/\theta_m B)$ is the gradient of the f-m water velocity (assuming the velocity is linearly distributed and zero in the middle of the matrix).

Both Schemes (3) and (4) were tested against the analytical solution for solute transport in fratured porous media with parallel fractures derived by Sudicky and Friend (1982). Because no

water flow occurs through the fracture-matrix interface in this case, as expected, both methods (i.e., dual-continuum particle tracker [DCPT] with Eq. (3) and DCPT with Eq. (4) in Figure 1) predict breakthrough curves that are almost identical to the analytical solution.
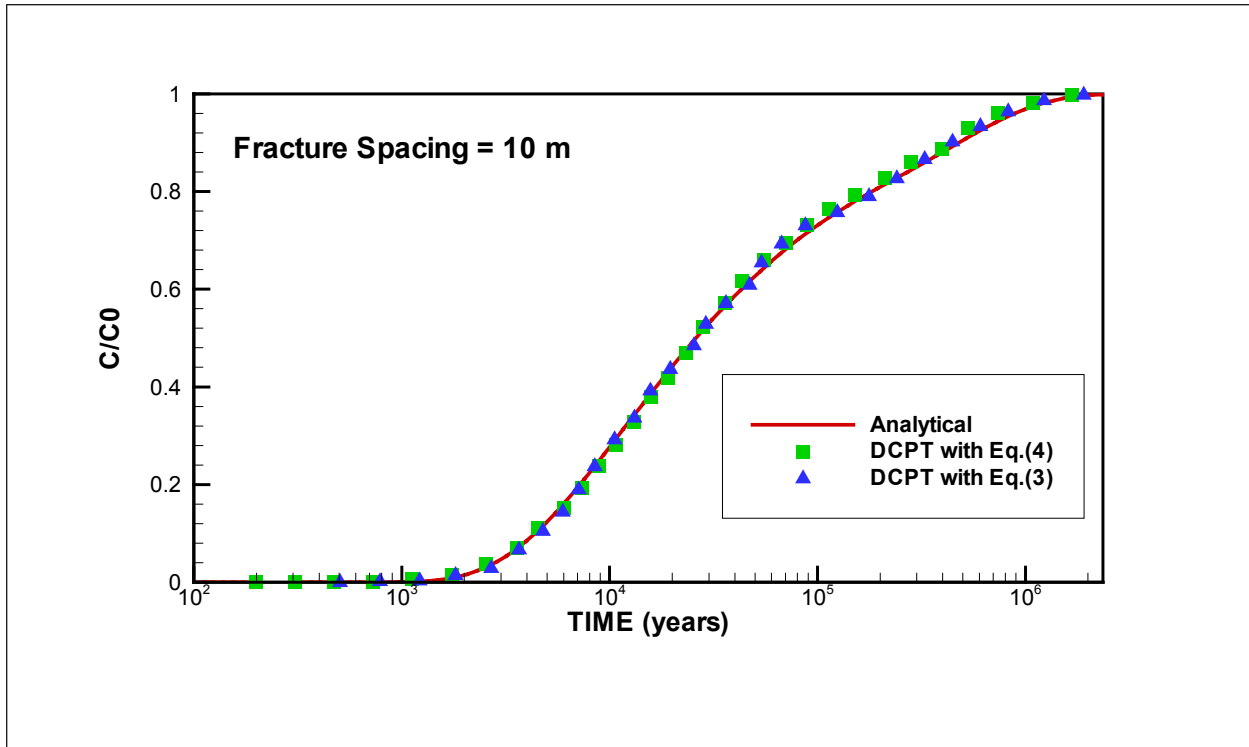


Figure 1. Comparison of particle tracking methods against the analytical solution (no water flow through the fracture-matrix interface)

The second test case considered a vertical column consisting of multiple layers of tuffs. A conservative tracer was released in the middle elevation of the column, and the cumulative mass breakthrough the bottom was simulated. The water flow was steady state, and significant water flow through the fracture-matrix interface occurred. Because no analytical solution is available for this case, the multiple interactive continuum (MINC) (Pruess and Narasimhan, 1985) numerical model was considered to be accurate, since it uses multiple matrix grid cells to capture the detailed processes within the matrix. The numerical code, T2R3D (Wu and Pruess, 2000), was used to perform the simulations. Ten matrix cells per each fracture cell were used in the MINC model. A dual-permeability (2k) model (one matrix cell per each fracture cell) was also included as a reference. In this comparison, the same steady state flow field was used in all simulations.

As shown in Figure 2, although the particle tracker with the previous scheme (Eq. 3) effectively solved the early breakthrough problem associated with the conventional dual-continuum model (e.g., T2R3D-2k), it does not compare well with the MINC model (e.g., T2R3D-MINC). Especially at late time, it may be even more inaccurate than the conventional dual-continuum model when significant water flow occurs through the fracture-matrix interface. On the other hand, the particle tracker with the new proposed scheme (Eq. 4) predicts almost identical

breakthrough curves as the MINC model (Figure 2). In other words, the particle tracker with the new scheme can attain accuracy similar to the MINC model in predicting the breakthrough curves but without using MINC's additional matrix grid cells (9 in this case), provided that the flow fields are the same.
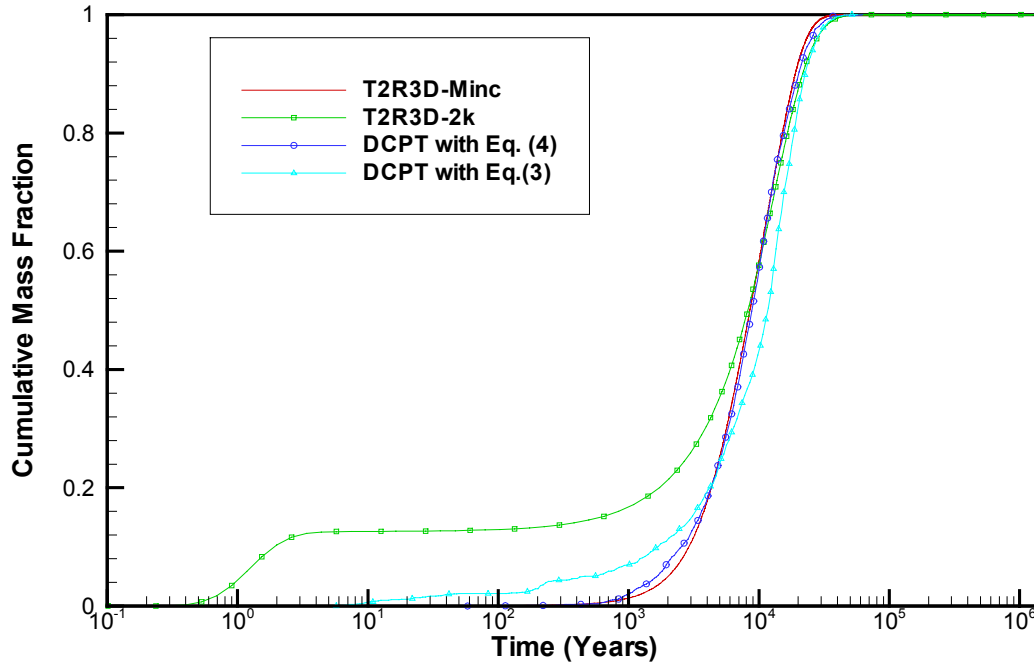


Figure 2. Comparison of particle tracking methods against the MINC numerical models (with significant water flow through the fracture-matrix interface)

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