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An improvement to DCPT:  
The particle transfer probability as a function of particle's age

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### Research Objectives

Multi-scale features of transport processes in fractured porous media make numerical modeling a difficult task of both conceptualization and computation. Dual-continuum particle tracker (DCPT) is an attractive method for modeling large-scale problems typically encountered in the field, such as those in unsaturated zone (UZ) of Yucca Mountain, Nevada. The major advantage is its capability to capture the major features of flow and transport in fractured porous rock (i.e., a fast fracture sub-system combined with a slow matrix sub-system) with reasonable computational resources. However, like other conventional dual-continuum approach-based numerical methods, DCPT (v1.0) is often criticized for failing to capture the transient features of the diffusion depth into the matrix. It may overestimate the transport of tracers through the fractures, especially for the cases with large fracture spacing, and predict artificial early breakthroughs. The objective of this study is to develop a new theory for calculating the particle transfer probability to captures the transient features of the diffusion depth into the matrix within the framework of the dual-continuum random walk particle method (RWPM).

### Approach

After a pulse of particles is injected into the fractures of a fracture-matrix system, the cloud of particles expands into matrix gradually due to mass transfer through the fracture-matrix interface. Although the range and the shape of the cloud are complicated for an arbitrary fracture-matrix system, both of them are transient. In terms of random walk method, all particles of that pulse will be confined within a limited range in the matrix. This range can be called as the activity range of a particle which can be defined as the range in the matrix such that the probability of finding the particle outside the range is practically zero. The activity range of a particle is a function of the time elapsed since the pulse to which the particle belongs is injected, which can simply be tracked as the particle's age in a dual-continuum RWPM. Consequently, the particle transfer probability of a particle is a function of the particle's age. A quantitative relationship between the activity range of a particle and the particle's age is derived based on an analytical solution for a system of parallel-plate fractures separated by porous rock responding to a pulse injection in the fractures. The new method is implemented in DCPT v2.0.

### Accomplishments and Significance of findings

The new method has been verified against analytical solutions for variety fracture spacing (Figure 1). Both old (DCPT v1.0) and new schemes (DCPT v2.0) predict the

breakthrough curves that agree well with the analytical solutions for the case with a fracture spacing of 1 m. However, for the case which has a larger fracture spacing of 10m, the old scheme seriously overestimates the breakthrough at early times (Figure 1). On the other hand, the new scheme predicts the breakthrough curves that are almost identical to the analytical solutions for both cases (Figure 1). Thus the new scheme effectively solves the problem of capturing the transient features of the diffusion depth into the matrix using only one matrix block to represent the matrix. It does not assume a passive matrix medium (as required by a residence-time particle tracking approach) and can be applied to the cases where global water flow exists in both continua. The method is also used to calculate the breakthrough curves of radionuclides from a potential repository to the ground water table in Yucca Mountain. The calculation demonstrates the effectiveness of this new technique for simulating of the 3-D, mountain-scale transport in a heterogeneous, fractured porous medium under variably saturated conditions. The results show that the effects of the transient features of the diffusion depth into matrix on the breakthrough of radionuclides are significant.

#### **Related publication**

Pan, L., and G. S. Bodvarsson, Modeling transport in fractured porous media with random-walk particle method: The transient activity range and the particle transfer probability, Water Resources Research, 2001 (submitted).

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Figure 1 Predicted breakthrough curves by DCPT v1.0, DCPT v2.0, and the analytical solutions for the case with a smaller fracture spacing of 1 m and the case with a larger fracture spacing of 10 m, respectively.

