Solute Transport in Fractured-Porous Media:
Dual Porosity Simulations with MT3D

Christopher J. Neville
S.S. Papadopulos & Associates, Inc.
Last update: July 14, 2006

1. Introduction

These notes describe an approach for simulating transport in porous fractured rocks using MT3D. The approach is relatively simple but approximates the important process of diffusive exchange of solutes between the fractures and porous matrix.

Fractured-porous media have two distinct pore spaces: the voids space between the fracture walls; and the pore space in the intact matrix blocks. The void space of the fractures may represent only a relatively small fraction of the total volume of the medium [typical fractions range from 0.01 to 0.1% of the total volume]. In contrast, the porosity of the intact matrix blocks may be relatively high. For example, tests on intact samples of the Lockport Dolomite indicate matrix porosities in the range of 1 to 10%.

Distinct fracture and matrix porosities generally do not have to be considered in the context of groundwater flow simulation. The effective hydraulic conductivity of an open fracture is generally much larger than the conductivity of intact matrix blocks and flow will occur primarily in the fracture network. Because there is effectively only one porosity that is active with respect to flow, flow in a fractured-porous medium can be simulated using an Equivalent Porous Medium (EPM) approach. In this approach, the fracture network is replaced by porous medium with the same effective hydraulic conductivity, defined as the conductivity that yields the same discharge as the fracture network under the same bulk hydraulic gradient. This approach has been adopted to simulate groundwater flow for many applications.

Although the matrix may not play a significant role with respect to flow, it may be very significant with respect to solute transport. The pore space in the matrix blocks represents a significant reservoir into and out of which solute can diffuse from the fractures. Conventional porous media transport simulators do not represent the diffusive mass exchange between the fractures and the matrix; therefore, they cannot be applied for EPM modeling of solute transport in fractured-porous media. Several codes are available that are capable of simulating coupled transport between a network of discrete fractures and porous blocks (for example, TRAFRAP, STAFF3D, FRACTRAN, FRAC3DVS). However, even in cases where the geometry and properties of the fracture network is known, the computational demands are very high and simulation of large-scale sites is not feasible. This note describes an alternative *dual-domain* approach implemented in MT3D that retains the simplicity of the EPM approach but approximates the diffusive exchange of solutes between the fractures and porous matrix.

2. MT3D dual porosity approach

The most recent versions of MT3D (MT3DMS and MT3D[99]) support dual domain modeling, using the first-order mass transfer coefficient approach (FOMT). It is perhaps simplest to appreciate the FOMT model by examining the one-dimensional forms of the governing equations for the concentrations in the mobile and immobile domains. For simplicity we will neglect any sorption or transformation reactions.

The statement of mass conservation for solute in the mobile domain is:

$$\theta_m \frac{\partial C_m}{\partial t} = -q \frac{\partial C_m}{\partial x} + \theta_m D_{Lm} \frac{\partial^2 C_m}{\partial x^2} - \varsigma \left(C_m - C_{im} \right) \tag{1}$$

The statement of mass conservation for solute in the immobile domain is:

$$\theta_{im} \frac{\partial C_{im}}{\partial t} = \varsigma \left(C_m - C_{im} \right) \tag{2}$$

where:

C_m : concentration in the mobile domain [ML^{-3}]
C_{im} : concentration in the immobile domain [ML^{-3}]
q : Darcy flux [LT^{-1}]
θ_m : porosity of the mobile zone (fractures) [-]
θ_{im} : porosity of the immobile zone (matrix blocks) [-]
ζ : first-order mass transfer coefficient [T^{-1}]

The linking term $\zeta\,(C_m\text{-}C_{im})$ appears in both (1) and (2), but with opposite signs. This reflects the fact that the mass flux from the mobile region to the immobile region represents a sink from the perspective of the mobile region, while at the same time acting as a source to the immobile region.

As incorporated in (1) and (2), the mass transfer between the mobile and immobile regions is treated phenomenologically. That is, the mass transfer coefficient appears to be a "curve-fitting" parameter with little underlying physical significance. At first glance it appears that the value of ζ cannot be determined *a priori*, and therefore the whole first-order approach has little predictive capabilities.

3. Application of the FOMT approach for fractured-porous media

The FOMT approach is not necessarily merely phenomenological when applied to represent transport in fractured-porous media – at least for idealized systems. Exact relations for the diffusive exchange between fractures and matrix blocks consisting of uniform slabs or spheres have been developed. Genuchten and Dalton (1986) and Sudicky (1990) have shown that with some further simplifying assumptions, simple analytical expressions can be derived for ζ such that the first-order mass transfer coefficient approach effectively mimics the slab and sphere models.

van Genuchten and Dalton's expressions for the first-order mass transfer coefficient are given below.

1. For parallel slabs:

$$\varsigma = \frac{3\theta_{im} D_{im}^{*}}{B^{2}} \tag{3}$$

2. For spheres:

$$\varsigma = \frac{15\theta_{im} D_{im}^{*}}{r_{o}^{2}} \tag{4}$$

where:

D^*_{im} : effective diffusion coefficient for the immobile zone $[L^2T^{-1}]$
B : slab-thickness [L]
r_0 : sphere radius [L]

In the next section, we consider an example application in which the results of an exact model for the slab geometry are compared with those from FOMT calculations. In the first analysis, the FOMT solution is evaluated with an analytical implementation of the first-order model. In the second analysis, the calculations are repeated using the FOMT model implemented in MT3D.

4. Example application

To quantitatively examine the reliability of the FOMT approach for simulating solute transport in fractured media we consider an example application in which the results of an exact model for transport in discretely-fractured porous media are compared with those from FOMT calculations. We consider the highly idealized situation of a set of fractures with uniform aperture separated by uniform slabs of intact rock. In the first analysis, the FOMT solution is evaluated with an analytical implementation of the first-order model. In the second analysis, the calculations are repeated using the FOMT model implemented in MT3D.

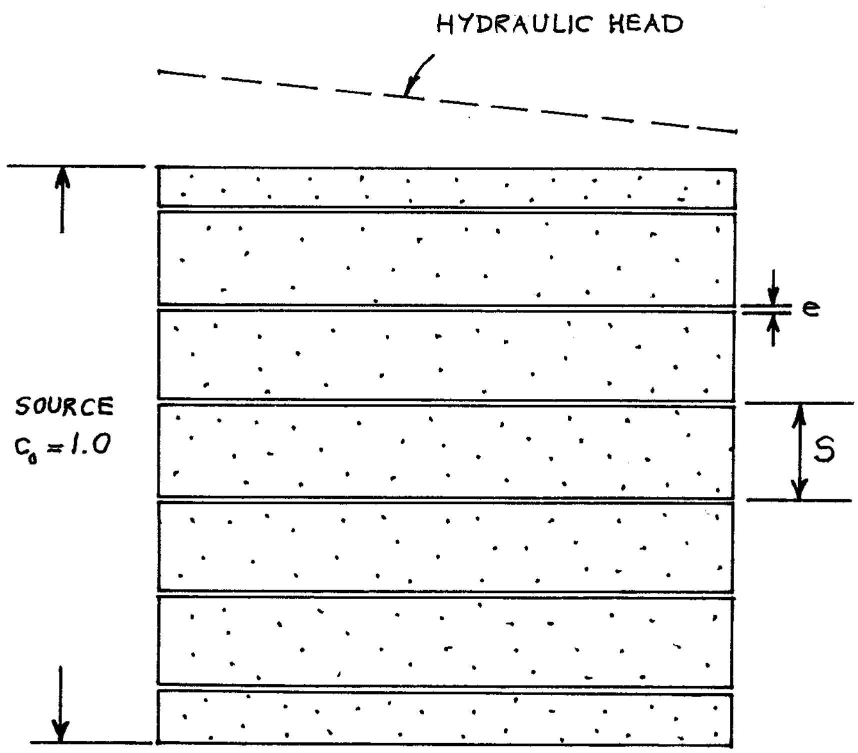

Figure 1. Definition sketch

Exact solution

Benchmark results are obtained using the exact analytical solution for transport along a set of discrete fractures with porous matrix slabs presented by Sudicky and Frind (1982). The solution is implemented in the code CRAFLUSH2. The calculated concentration profiles along the fractures are shown in Figure 2.

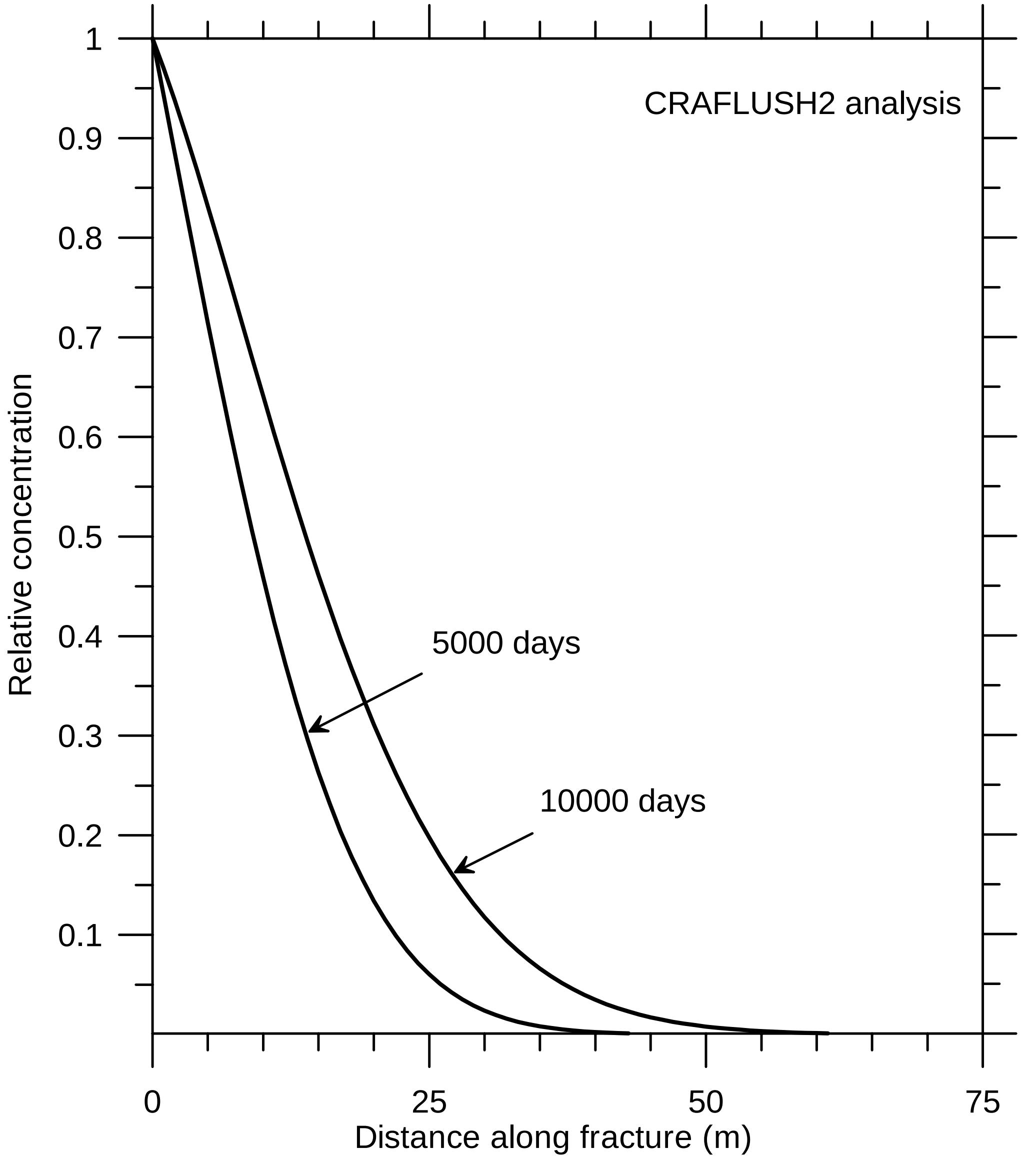

Figure 2. Results from discrete fracture analysis

FOMT results

For the second analysis, we simulate the discrete fracture system as an equivalent dual porosity medium, using the FOMT approach implemented in the MPNE1D analytical solution (Neville et al., 2000) and the numerical transport model MT3DMS. To use the FOMT approach we require estimates of the following parameters:

- Mobile porosity;
- Immobile porosity; and
- The first-order mass transfer coefficient.

The mobile porosity is calculated as:

$$\begin{aligned}\theta_m &= \frac{e}{S+e} \\ &= \frac{\left(100\times10^{-6}\,m\right)}{\left(1.0\,m\right)+\left(100\times10^{-6}\,m\right)} = 9.999\times10^{-5}\end{aligned}$$

The total porosity is given by:

$$\begin{aligned}\theta &= \theta_m + \theta_{im} \\ &= 9.999\times10^{-5} + 0.01 = 1.010\times10^{-2}\end{aligned}$$

Therefore, the ratio of the mobile porosity to the total porosity is:

$$\begin{aligned}\phi &= \frac{\theta_m}{\theta} \\ &= \frac{\left(9.999\times10^{-5}\right)}{\left(1.010\times10^{-2}\right)} = 9.900\times10^{-5}\end{aligned}$$

Several researchers have developed exact relations for the diffusive exchange between fractures and matrix blocks consisting of uniform slabs or spheres. van Genuchten and Dalton (1986) and Sudicky (1990) have shown that with some further simplifying assumptions, simple analytical expressions can be derived for ζ such that the first-order mass transfer coefficient approach effectively mimics the slab and sphere models. van Genuchten and Dalton’s expression for the first-order mass transfer coefficient for transport in a set of parallel slabs is:

$$\varsigma = \frac{3\theta_{im} D_{im}^{*}}{B^{2}}$$

In this equation we have:

θ_{im} porosity of the immobile zone (porosity that is occupied by the matrix slabs) [-]

D^*_{im} : effective diffusion coefficient for the immobile zone [L^2T^{-1}]

B : slab half-thickness [L]

Using the parameters assumed previously we calculate:

$$\varsigma = \frac{3(0.01)(1.380\times10^{-5}\, m^2/d)}{(1.0\,m/2)^2} = 1.656\times10^{-6}/d$$

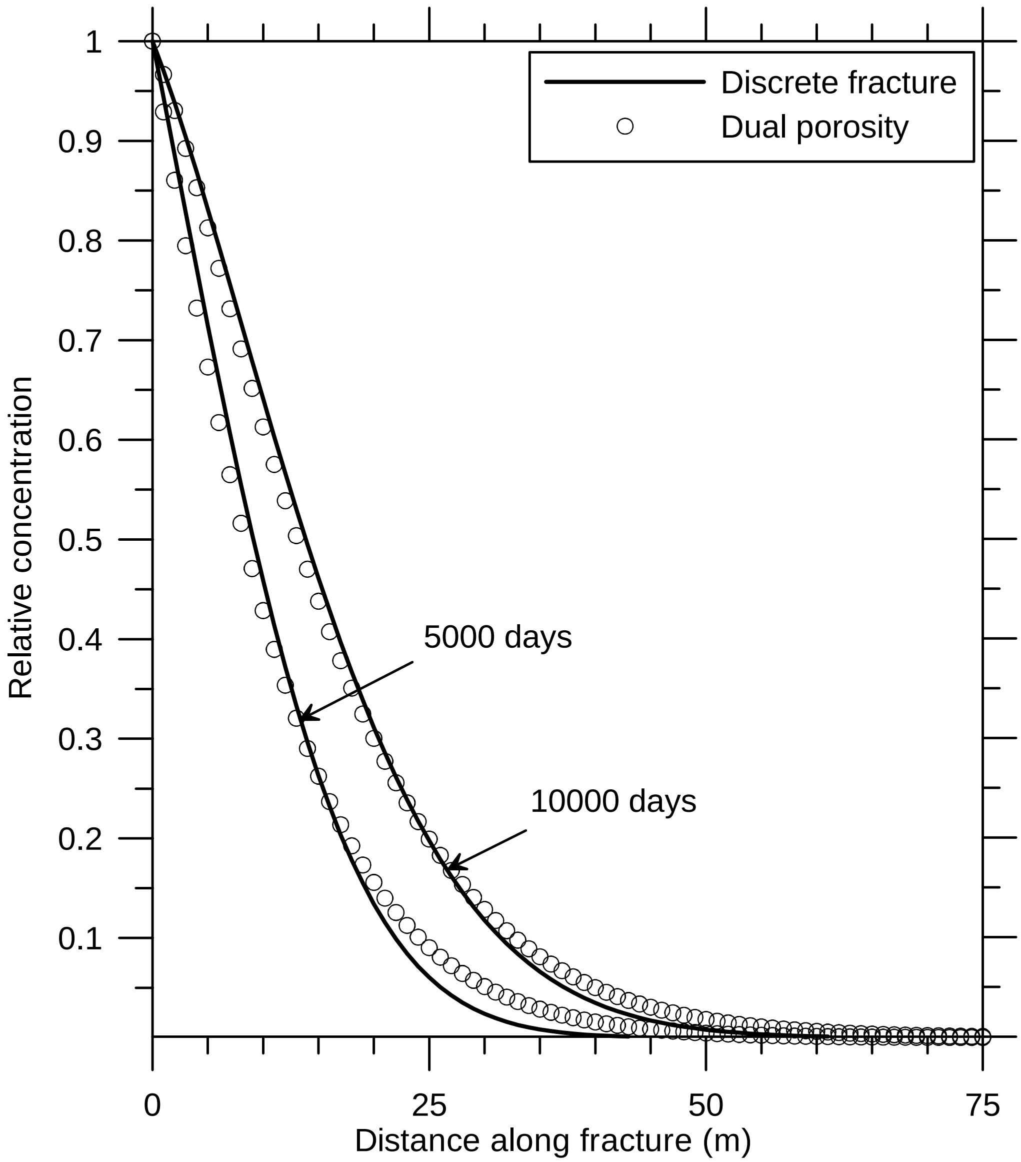

Figure 3. Results from analytical dual porosity analysis

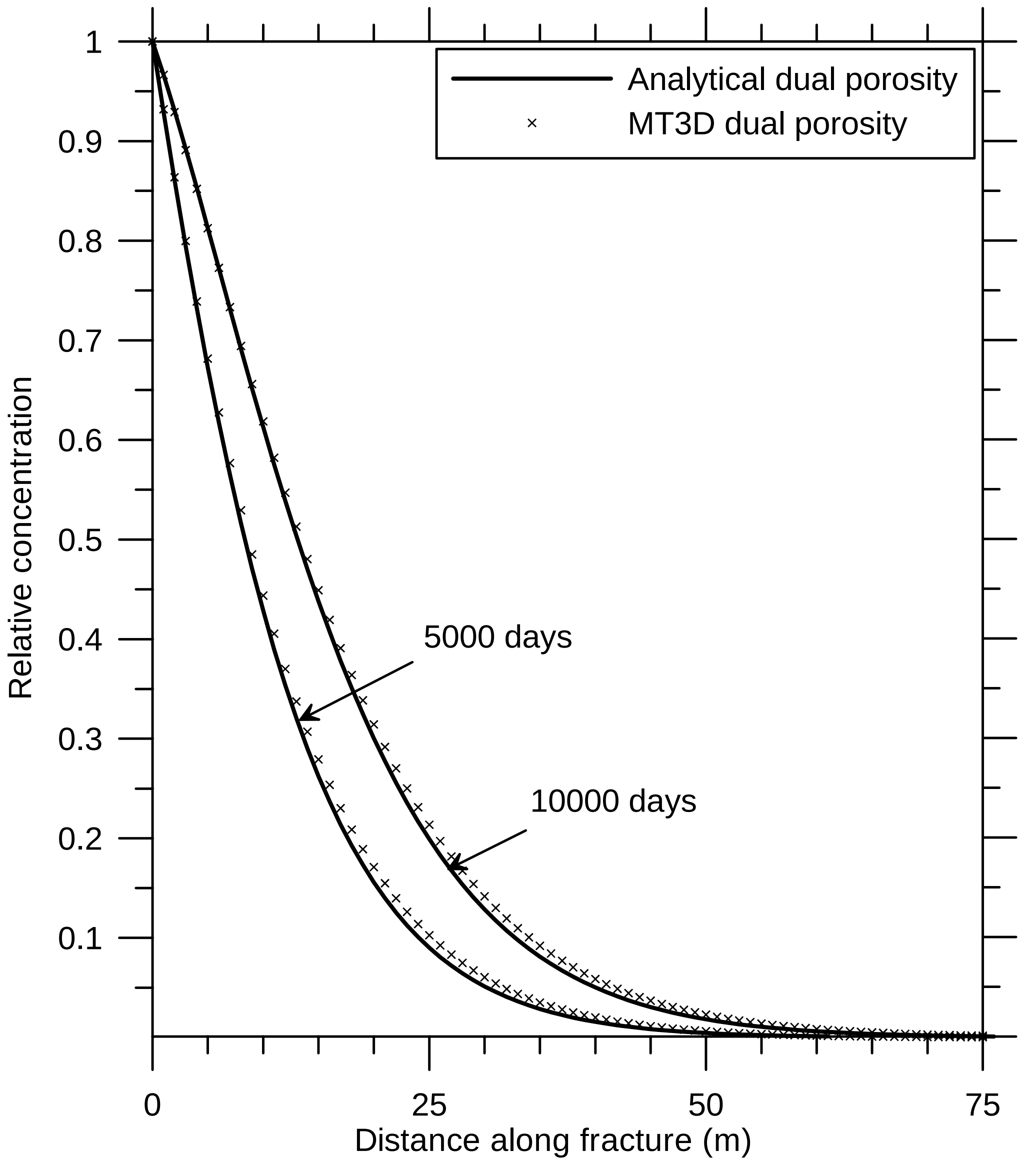

Figure 4a. Results from MT3D dual porosity analysis

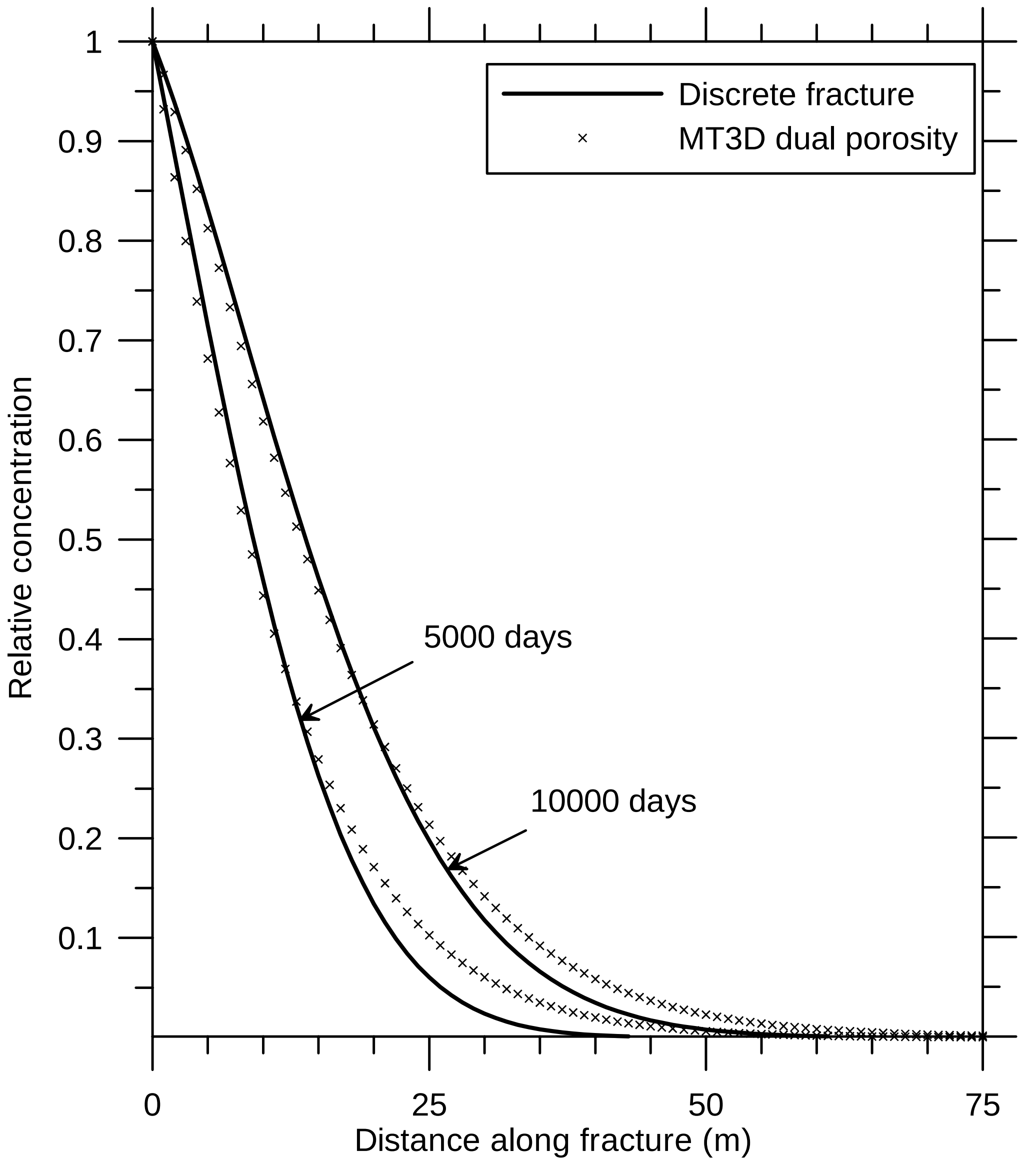

Figure 4b. Results from MT3D dual porosity analysis

5. Conclusions

In this note we have compared the results of an exact solution for transport in a set of ideal discrete fractures separated by porous matrix blocks with results obtained using a first-order mass transfer coefficient approach (FOMT). The principal findings of the analysis are summarized below:

1. The results of the benchmarking problem confirm that the FOMT formulation can match the exact results from a discrete fracture analysis.

2. The dual porosity option has been implemented correctly in MT3D.

3. The general trend of the MT3D results confirms that the FOMT formulation adopted with MT3D can be used to simulate transport along a simple system of discrete fractures.

A traditional objection to the use of the FMOT approach is its phenomenological basis. Simply put, it has been typically thought that the immobile porosity and first-order mass transfer coefficient are fitting parameters that cannot be estimated independently. In this note we have demonstrated that the FOMT approach is not necessarily merely phenomenological when applied to represent transport in fractured-porous media – at least for idealized systems. Exact relations for the diffusive exchange between fractures and matrix blocks consisting of uniform slabs or spheres have been developed. Genuchten and Dalton (1986) and Sudicky (1990) have shown that with some further simplifying assumptions, simple analytical expressions can be derived for ζ such that the first-order mass transfer coefficient approach effectively mimics the slab and sphere models.

6. References

Neville, C.J., M. Ibaraki, E.A. Sudicky, 2000, Solute Transport with Multiprocess Nonequilibrium: A Semi-Analytical Solution Approach, *Journal of Contaminant Hydrology*, 44, pp. 141-159.

Sudicky, E.A., 1990: The Laplace transform Galerkin technique for efficient time-continuous solute of solute transport in double-porosity media, *Geoderma*, *46*, pp. 209-232.

Sudicky, E.A., and E.O. Frind, 1982: Contaminant transport in fractured porous media: Analytical solutions for a system of parallel fractures, *Water Resources Research*, *18*(6), pp. 1634-1642.

van Genuchten, M.T., and F.N. Dalton, 1986: Models for simulating salt movement in aggregated field soils, *Geoderma*, *48*, pp. 165-183.

Zheng, C., 2002: MT3D^{99}: A Modular 3D Multispecies Transport Simulator, (Version SP-4) S.S. Papadopulos & Associates, Inc., Bethesda, MD.