Effect of Small-Scale Fractures on Flow and Transport Processes at Yucca Mountain, Nevada

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1. Introduction

Various conceptual models have been proposed and tested for modeling fracture-matrix interaction in Yucca Mountain site characterization studies (Doughty, 1999). Currently, the most widely used model is the dual-permeability approach. This is because the dual-permeability model has proved to be capable of matching many types of field-observed data (e.g., Wu et al. 1999). Secondly, net-infiltration rates at the site are so low (on the order of millimeters/year) or close to saturated matrix hydraulic conductivity that global matrix-matrix flow can no longer be ignored. Recent field observations and, in particular, fracture mapping data collected along the walls of the underground tunnels, reveal a significantly large variety in fracture length from centimeters to tens of meters. However, these large numbers of small fractures have not been considered in most previous modeling studies. This may result from the inability of the currently used dual-permeability model to include the effects of small-scale fractures.

To overcome the limitations of the dual-permeability approach, we propose a triple-continuum conceptual model to investigate the impact of small-scale fractures on flow and transport processes in fractured rocks. This new conceptual model subdivides fractures into two types: large-scale and small-scale. Large-scale fractures are those responsible for global connections; small-scale fractures are those that provide large-fracture storage space and enhance the local connections to the matrix system *without* contributing to global flow or transport. The model formulation uses three sets of conservation equations to describe flow and transport processes at each location of the system, for the two-fracture and one-matrix systems, respectively. The proposed triple-continuum model has been implemented into a numerical model and applied to field problems at Yucca Mountain.

This work consists of (1) development of a triple-continuum geological conceptual model; (2) derivation of a mathematical model and numerical formulation for

the proposed triple-continuum concept; and (3) model application to the Yucca Mountain site. The primary objectives of this study are to propose a new and more appropriate conceptual model for better handling fracture-matrix interactions and to evaluate effects of small-scale fractures on flow and transport processes in the unsaturated zone (UZ) of Yucca Mountain.

2. Conceptual Model and Mathematical Formulation

We conceptualize a fracture-matrix system to consist of two types of fractures, "large" fractures and "small" fractures, as well as porous-medium rock matrix. Large fractures are defined as those that contribute to global flow and transport through the model domain and small fractures are ones that are not directly connected globally but well-connected to both large fractures (i.e., globally connected) and matrix blocks. These small fractures have more storage space or bigger porosity than large fractures. In addition, small fractures that are not connected with large fractures and isolated within the matrix are considered part of the matrix system. The triple-continuum model is an extension of the dual-permeability concept by adding one more connection between large fractures and matrix blocks through small fractures.

Figure 1 presents an illustration for triple-continuum approximation to one-dimensional large-fracture and small-fracture and rock matrix systems, respectively. The same conceptualization (Figure 1) can be extended to a two- or three-dimensional fractured-matrix system. Note that the triple-continuum concept is not limited to such a regular idealization (Figure 1). In general, actual configuration and distribution of both small and large fractures can be stochastic and handled using an approach similar to the MINC methodology (Pruess, 1983), as long as such a distribution pattern is known. In the triple-continuum approach, processes of flow and transport in fractured rocks are described separately, using a triplet of governing equations for the two-fracture and matrix system. This conceptualization results in a set of partial differential equations for flow and transport in each continuum of fractured media, which are in the same form as that for a single-continuum porous medium. Transport of each component in a liquid-gas,

two-phase nonisothermal system within the two fracture continua or matrix continuum can be described using mass- and energy-balance equations.

The numerical implementation of the triple-continuum model is based on the framework of the TOUGH2 code (Pruess, 1991; Wu and Pruess, 2000). The component mass- and energy-balance equations are discretized in space using the integral-finite-difference method in a porous and/or fractured medium. The time discretization is carried out with a backward, first-order, finite-difference scheme. In addition, we use the MINC techniques directly from Pruess (1983) for handling flow and interactions between large fractures and matrix. However, this work introduces one additional continuum, small fractures. In evaluating the "flow" terms between small fracture to large fracture or small fracture to matrix connections, we need additional geometric parameters, such as interface areas and characteristic lengths for these connections. It is further assumed in the numerical formulation that small fractures are represented using one cell, locally interacting with large fracture and matrix systems. Table 1 summarizes the equations needed for determining characteristic distances in calculating flow between three continua for the cases of regular one-, two- and three-dimensional large fracture networks, and uniform distributions of small fractures, as shown in Figure 1. In deriving these equations (Table 1) for calculating "flow" distance between two fracture and matrix systems, we use the same quasi-steady state flow assumption as the Warren-Root (1963) model. Interface areas between large fractures and the matrix and between large fractures and small fractures are treated using the geometry of the large fractures or bulk connection areas. For connection between small fractures and matrix, however, actual interface areas are used.

Table 1 Characteristic distances* for evaluating flow terms between two fracture and matrix systems.

Large-Fracture	Dimensions of matrix blocks	Characteristic Dimension (m) of large fractures	Characteristic F-M distances (m)	Characteristic dimension (m) of small fractures	Characteristic F-f distances (m)	Characteristic f-M distances (m)
1-D	A	$l_F = \mathrm{A}$	$l_{FM} = l_F / 6$	$l_f = \mathrm{a}$	$l_{Ff} = l_x / 2$	$l_{fM} = l_f / 6$
2-D	A B	$l_F = \dfrac{2\mathrm{AB}}{\mathrm{A}+\mathrm{B}}$	$l_{FM} = l_F / 8$	$l_f = \dfrac{2\mathrm{ab}}{\mathrm{a}+\mathrm{b}}$	$l_{Ff} = \dfrac{l_x + l_y}{2}$	$l_{fM} = l_f / 8$

3-D	A B C	$l_F = \frac{2ABC}{A+B+C}$	$l_{FM} = l_F/10$	$l_f = \frac{2abc}{a+b+c}$	$l_{Ff} = \frac{l_x + l_y + l_z}{2}$	$l_{fM} = l_f/10$

* Note in Table 1, A, B and C are dimensions of matrix blocks along x, y and z directions, respectively; a, b and c are fracture-spacings of small fractures along x, y and z directions, respectively; subscript F represents large-fracture, f for small-fracture and M for matrix systems, respectively.

4. Model Application

To demonstrate application of the triple-continuum model to flow and transport processes, we present a 3-D modeling study of small-fracture effects, based on the site-scale unsaturated zone flow model for the total system performance assessment (TSPA) (Wu et al., 2000). The 3-D UZ model grid (Figure 2) has 1,324 mesh columns of fracture and matrix continua and 37 computational grid layers vertically, resulting in 145,640 gridblocks and 492,098 connections for a triple-continuum grid. Fracture-matrix interactions in the 3-D modeling are handled using the triple continuum and compared with the results from the dual-permeability model. An active fracture model (Liu et al., 1998) is also integrated into these two models to represent fingering flow effects through fractures.

The ground surface and water table are taken as the model top and bottom boundary, respectively, and both are treated as Dirichlet-type boundaries. All the lateral boundaries (Figure 1) are treated as no-flow (laterally closed) boundaries. In addition, surface net infiltration is applied to fracture blocks below the top boundary as source terms with the modern mean infiltration map, which is spatially varying and estimated by the US Geological Survey (USGS) scientists (Hevesi and Flint, 2000) for the site.

Hydraulic properties for large fracture and matrix for the triple-continuum model are the same as those for the dual-permeability UZ flow model (Wu et al., 2000), and

small-fracture properties are estimated using an inverse modeling approach along with field-measured matrix moisture data. In addition, the present triple-continuum model incorporates the permeability-barrier model for modeling the occurrence of perched water, as observed in the UZ (Wu et al., 2000).

Simulation results of steady-state flow, obtained with the triple-continuum model, are checked in terms of (1) comparisons with measured moisture data and (2) the match with observed perched-water bodies. In addition, we find a very similar flow pattern, as predicted using the triple- or dual-continuum models under the same infiltration scenario and boundary conditions. This may indicate that small fractures have little impact on steady-state global unsaturated flow because they are not globally connected.

In addition to the flow simulation with the triple-continuum concept, modeling results for tracer/radionuclide transport are presented with the steady-state 3-D flow field, using a conservative (technetium) and a reactive (neptunium) radionuclide. Transport simulation is conducted using a decoupled version of the T2R3D code (Wu and Pruess, 2000). The two radionuclides are treated as nonvolatile and are transported only through the liquid phase, with radioactive decay and mechanical dispersion ignored. A constant molecular diffusion coefficient of 3.2×10^{-11} (m^2/s) is used for matrix diffusion of the conservative component, and 1.6×10^{-10} (m^2/s) is used for the reactive component. For ^{237}Np, K_d values are set to 4 and 1(cc/g) for zeolitic and nonzeolitic matrix, respectively. For a conservative tracer, K_d is set to zero. All transport simulations were run to 1,000,000 years under steady-state flow and constant initial source concentration conditions at the repository.

Tracer transport times (traveling since release from the repository to the water

table) can be used as a measure of transport behavior at the Yucca Mountain site and is analyzed using a cumulative breakthrough curve at the water table. The breakthrough curve here is defined as a ratio of the cumulative mass of a radionuclide arriving at the water table over time to the total initial mass of the component at the repository as the function of time. Figure 3 compares simulation results from the two fracture-matrix conceptualizations, i.e., dual-permeability and triple-continuum models, and shows a significant difference in predicted cumulative breakthrough curves between the two models. For example, there is a one-order-of-magnitude difference in 20% breakthrough times for the nonsorbing radionuclide Tc. Even for the sorbing radionuclide Np, the 20% breakthrough times, obtained with the triple-continuum model, gets doubled.

Results in Figure 3 indicate that the conceptual model for fracture-matrix interactions is very important for radionuclide-transport simulation and should be selected appropriately. Note that Figure 3 shows longer transport times by the triple-continuum model than those by its counterpart, the dual-permeability model. This is because the triple-continuum model results in stronger interaction between fractures and matrix.

5. Summary and Concluding Remarks

A new triple-continuum conceptual model, a generalization of the commonly used dual-continuum model, has been applied to modeling fluid flow and radionuclide transport through heterogeneous fractured rock. The new conceptual model takes into consideration the fact that many of fractures in a subsurface system are not well-connected globally, but may still have an important effect on fracture-matrix interaction. It treats a fracture-matrix system by using two different types of fracture and one type of

matrix continuum. With this generalized multiple-continuum approach, the model formulation uses three parallel sets of conservation equations to describe flow and transport processes at each location of the system, for the two fracture and matrix systems, respectively.

The proposed triple-continuum model has been applied to field problems at Yucca Mountain. The 3-D modeling results obtained using the model indicate that small fractures can enhance fracture-matrix interaction and therefore have a significant impact on radionuclide transport in the UZ system, while their effects on unsaturated flow are insignificant.

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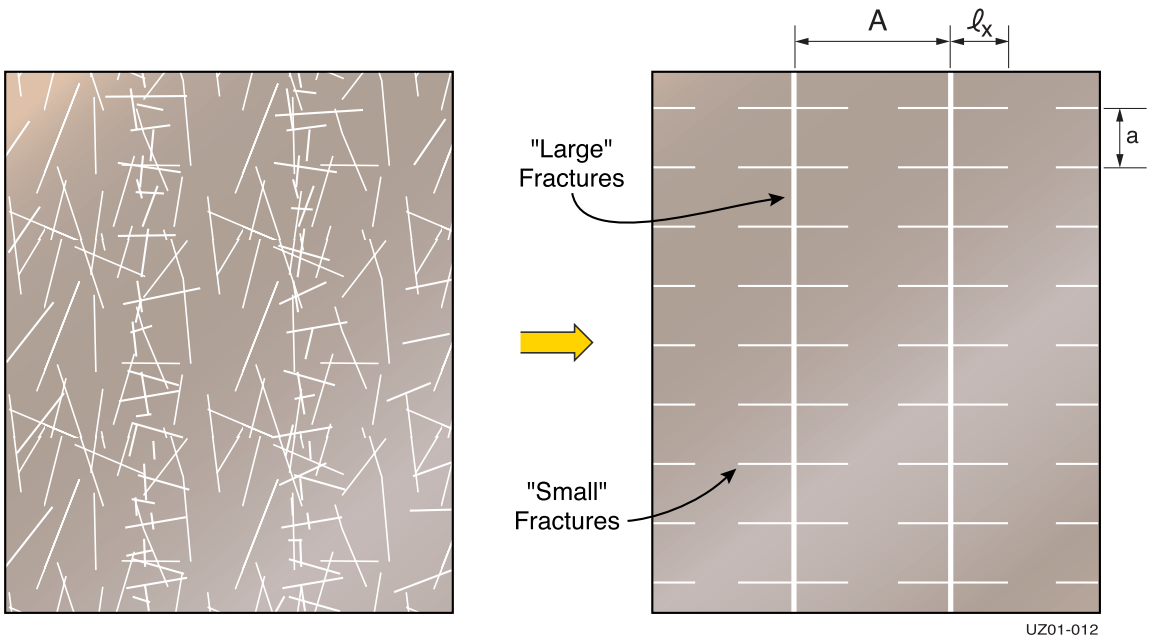

Figure 1. Basic conceptualization for triple-continuum approximation of one-dimensional large-fracture, small-fracture and rock matrix system.

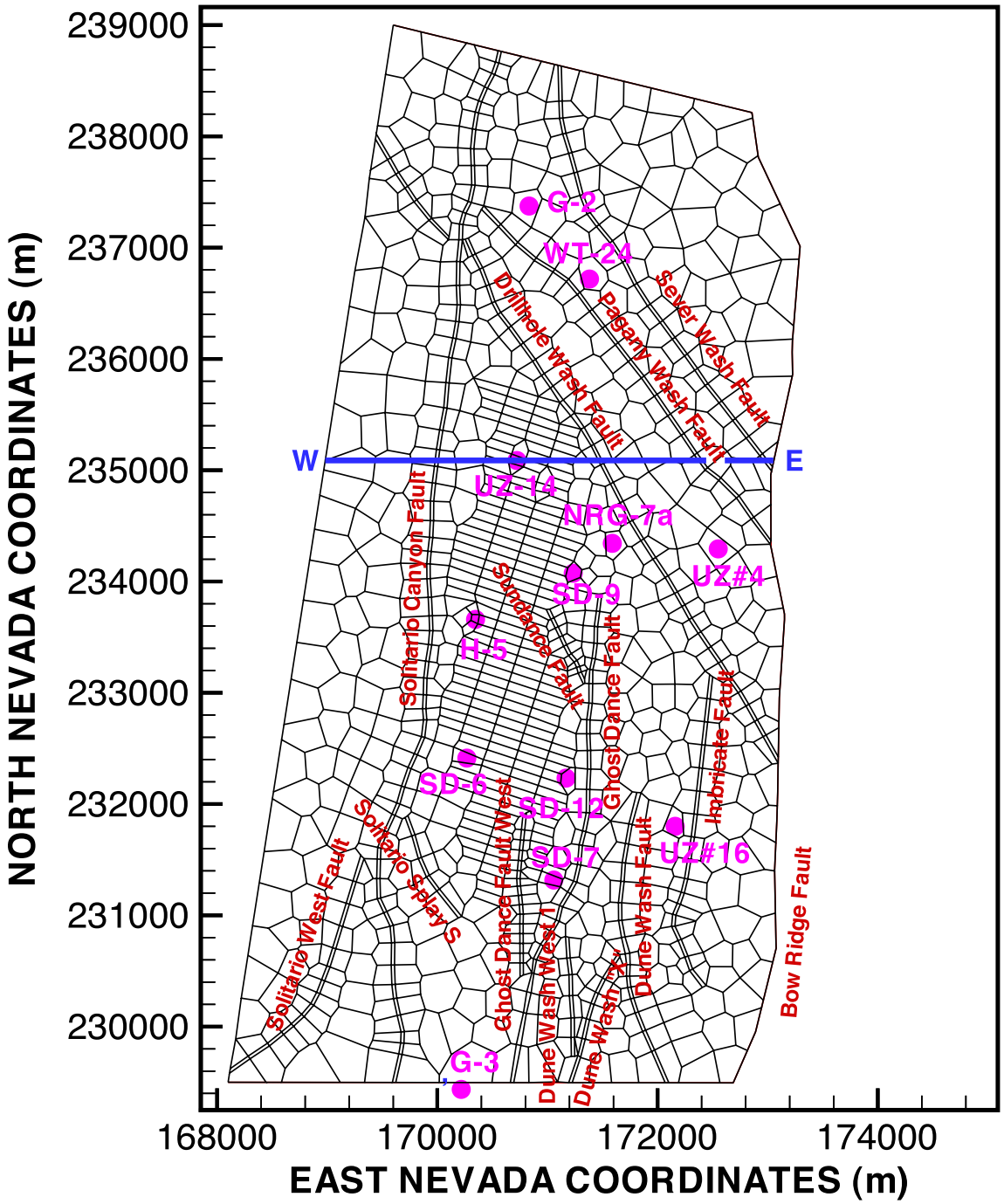

Figure 2. Plan view of the 3-D UZ model grid, showing the model domain, faults incorporated and borehole locations at the Yucca Mountain

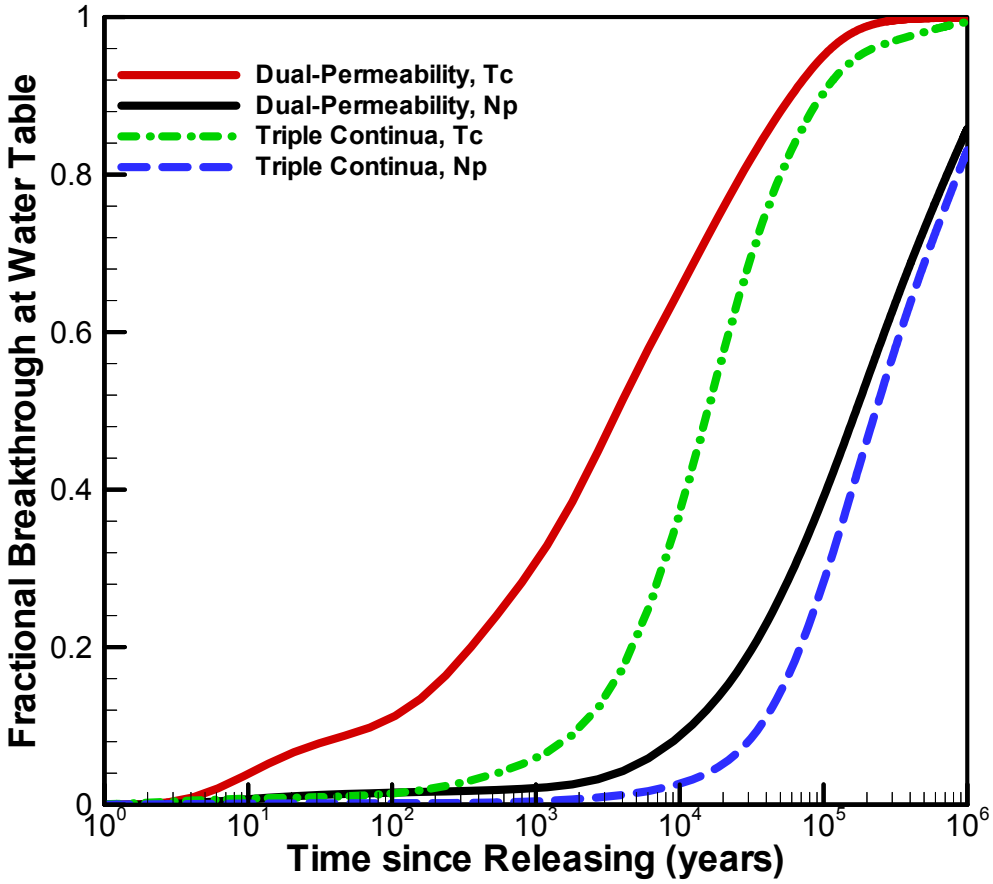

Figure 3. Comparison between cumulative breakthrough curves at the water table, simulated for conservative and reactive tracer transport from the repository with the dual-permeability and triple-continuum 3-D models, respectively,