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Comparison Between Dual and Multiple Continua Representations of Nonisothermal Processes in the Repository Proposed for Yucca Mounain, Nevada

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Introduction

Numerical simulation of nonisothermal, multiphase flow and associated reactive transport in fractured rock is an important tool for understanding geothermal systems, certain petroleum extraction processes, and, more recently, the behavior of potential geological repositories for high-level nuclear waste. A variety of approaches is available depending on how interactions between the fractures and matrix are modeled, and whether the fracture system is treated as an effective continuum or as a collection of discrete fractures. In studies of the high-level waste repository proposed for Yucca Mountain, Nevada, a dual continua representation has emerged as the standard approach for modeling processes in the unsaturated zone near emplacement tunnels (e.g. Wu and Pruess, 2000). In the dual continua approach, the fracture network is modeled as an effective continuum which interacts with a second continuum representing the matrix system. Contemporary incarnations of the dual continua approach have roots in the classical double-porosity models, but are more general in that coupled multiphase flow, heat transport, and solute transport are included. The primary motivation for the approach is to represent both the rapid response of the small-volume fractures and the slower response of the matrix system.

The chief limitation of the dual continua approach is that it neglects any gradients within a matrix block. The more general (and arguably more rigorous) multiple interacting continua (MINC) approach (Pruess and Narasimhan, 1985) allows for gradients in pressures, temperature, and concentrations in the vicinity of fractures. The essence of the MINC approach is that changes in fluid conditions will propogate more slowly in tight matrix blocks compared with the smaller volume fractures, an effect which causes local conditions in the matrix to be controlled by the proximity to a fracture. This phenomenology is captured in the MINC model by using several interacting continua to represent the matrix; all matrix material within a certain distance range from the fracture is lumped into one of the matrix continua. The dual continua model (DCM) is the special MINC case with only one matrix continuum. The dual continua is understood to be an adequate approximate for steady state or weakly transient systems, but the appropriateness of the approximation is more questionable for strongly transient systems that may have large gradients in the vicinity of fractures. However, few studies comparing the MINC and DCM representations at the field scale are available. In particular, studies specifically addressing the differences between MINC and dual continua representations of processes in the high-level waste repository proposed for Yucca Mountain are lacking. Such a comparison is given here. Specifically, MINC and dual continua represention of multiphase flow and reactive transport in the strongly heated repository near field are compared.

Model Description

The MULTIFLO code Version 1.5.2 (Lichtner, 1996; Lichtner and Seth, 1996; Painter et al., 2001) is used in this study. MULTIFLO simulates nonisothermal, multiphase flow and multicomponent reactive transport in fractured porous media. It is based on the integrated finite difference method, which allows for fully unstructured grids with arbitrary intercell connectivity. The dual continua approach is implemented explicitly. MINC models can be implemented through grid construction. Time stepping is fully implicit with newton iterations to resolve the nonlinearities. The general formulation and underlying mathematical models for the flow code are similar to that of Wu and Pruess (2000).

The two-dimensional computational domain (Figure 1) is a "chimney" type (tall and narrow). The base of the 450 meter high domain is at the water table, about 600 meters below the land surface. The emplacement tunnels for the proposed repository are about 300 meters above the water table. Horizontally, the domain spans one-half of the tunnel spacing (40.5 meters) with no-flow (symmetry) conditions on either side. Flow and heat transport processes within the tunnel are not modeled; instead, the heat eminating from the waste packages is applied as a time-dependent heat flux directly to the tunnel walls.

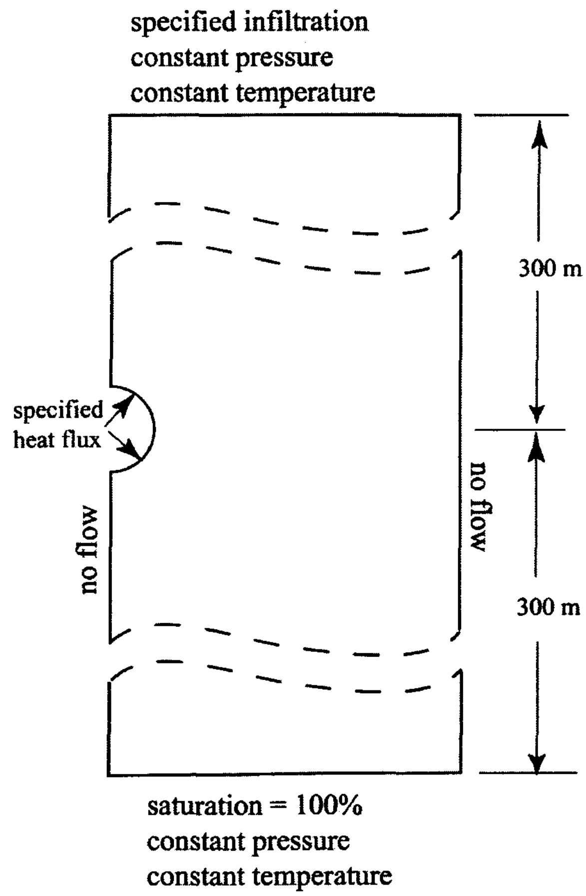

Figure 1: Two-dimensional computational domain (not to scale).

Thermal and hydrological property values for the major stratigraphic units considered in this work were taken from U.S. Department of Energy reports (2000). The model of van Genuchten (1978) is used to relate capillary pressures and liquid saturations. Capillary pressures and relative permeabilities for the fracture continuum and relative permeability for fracture-to-matrix flow are modified according to the active fracture model (Liu et al, 1998).

In the MINC and dual continua approaches the *primary grid* partitions the physical space into computational cells. Each cell in the primary grid is partitioned in turn by the *secondary grid* into fracture and matrix continua. The entire collection forms the aggregate or composite grid which is used in the numerical simulation. The MINC model used here has three matrix continua, resulting in an aggregate grid of size 3N+N=4N. A detail from the primary grid is shown in Figure 2. The unstructured grid is relatively fine in the vicinity of the emplacement tunnels and becomes much coarser away from the strongly heated region. The primary grid contains 690 computational cells.

Initial conditions for the thermal hydrology simulation were established by running an ambient non-heated simulation without the emplacement tunnel. Once this ambient run reached steady state, the computational cells in the tunnel region were removed and the heat turned on. The time dependent power applied to the tunnel walls is shown in Figure 3. Two scenarios were considered. In the first, the power output of the waste package was reduced by 75% to simulate the effects of forced ventilation during the first 50 years. This scenario is roughly consistent with time- and space-averaged values for ventilation efficiency as calculated from three-dimensional simulations incorporating self-consistent representation of ventilation processes (Painter et al, 2001). However, the ventilation effectiveness is dependent on time and position along the length of the emplacement tunnel. For this reason, a second scenario was considered. In the second scenario, the power was reduced by 50% during the first 50 years.

Fully coupled reactive-transport simulations were also performed. These highly idealized simulations were designed to test the sensitivity to choice of fractured rock conceptual model, and were were not intended to provide an accurate representation of the complex geochemical processes. Thus, one generic mineral was used as a proxy for the set of silica minerals present or expected to form at high temperatures near the emplacement tunnels. Other minerals were ignored. The principal phenomenon of interest is possible deposition of silica at the position of a boiling front in the fractured tuff rock.

Results

Liquid saturations in the matrix and fracture continua at the first node above the drift crown are plotted versus time in Figure 4. The heating scenario is the 75% reduction case. For both the MINC and dual continua approaches, the liquid saturation decreases strongly at 50 years corresponding to the end of the ventilation period. At late times (> 1000 years) the thermal pulse has passed and the liquid saturation returns to the initial conditions. In the intermediate period (50-1000 years), there are significant differences, with the MINC approach generally predicting dryer conditions. For the matrix system, the liquid saturation never drops below 20% in the dual continua simulation, whereas total dryout occurs in the matrix system over the period of 70-150 years in the MINC simulation. Rewetting also occurs earlier in the dual continua system. Results for the fracture system are generally similar to the matrix, with rewetting occuring at about 200 years in the dual continua simulation compared with 800 years in the MINC simulation.

Results for the alternative heating scenario of 50% heat reduction are shown in Figure 5. As with the 75% reduction case, significant differences between the MINC and dual continua approaches can be seen for limited times. In the case of the 50% reduction, large differences in saturation occur during the first 50 years and also in the rewetting time, again with the MINC approach predicting dryer conditions. This difference in saturation is partly due to differences in matrix pressure (right plot in Figure 5). During the strong heating period, the pressure in the matrix blocks increases in both the MINC and dual continua approaches. However, matrix pressures decay more slowly in the dual continua approach, and this pressure buildup raises the boiling temperature and allows significant liquid to remain in the matrix.

The amount of silica deposited in the fractures is also significantly different between the MINC and dual continua models. In simulation using the 50% heat reduction assumption, small amounts of silica are deposited in the fractures in a limited area about 2-3 meters above the emplacement tunnels. In the dual continua simulations, the silica occupies about 6% of the original fracture void space. In the MINC simulation, the fracture void space is reduced by only 2%. In either case, the reduction in porosity is too small to have significant effect on fracture permeability. The results are very insensitive to the actual mineral reaction rate because the mineral forming reaction is limited by the rate at which aqueous silica is brought to the boiling zone where deposition occurs. It is noted that fracture porosity in the Yucca Mountain region is uncertain and that smaller values of fracture porosity would result in a larger relative change in fracture porosity and permeability. Nevertheless, the conclusions about the MINC and dual continua models would remain unchanged.

Conclusions

1. The dual continua and MINC representations yield different results for fracture and matrix saturation under strongly heated conditions. However, the differences are significant only when temperatures are close to the nominal boiling temperature for water.
2. The MINC representation produces lower values for matrix and fracture saturation, as well as significantly longer periods of totally dry conditions at the tunnel crown.
3. The dual continua model predicts about three times as much silica deposition in fractures compared with the MINC representation. In either case, however, the amount of silica deposited is insignificant for the reference conditions considered here.
4. Because the dual continua representation results in wetter conditions as compared with the MINC model, the dual continua appears to be a conservative assumption from the perspective of repository performance assessment. However, studies aimed at comparing simulation models with the results of thermal hydrology experiments may benefit from MINC type models.

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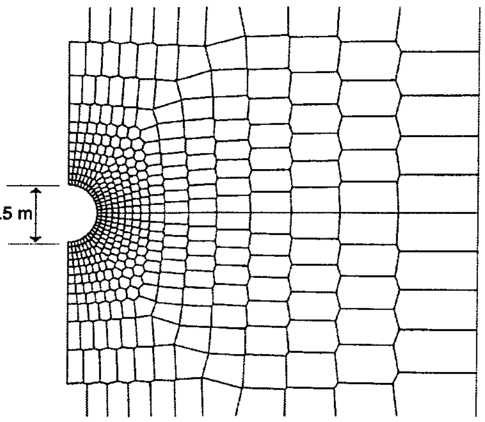

Figure 2. Detail from the primary grid.

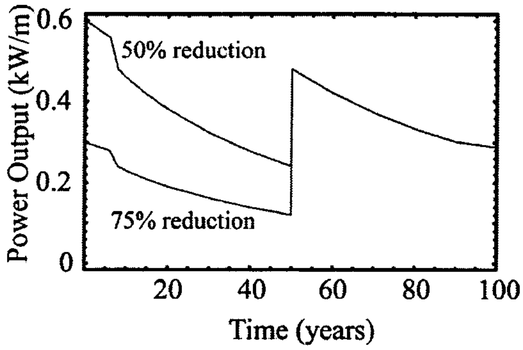

Figure 3. Heat load at the tunnel wall versus time after emplacement for different assumptions about ventilation effectiveness during the 50 year ventilation period.

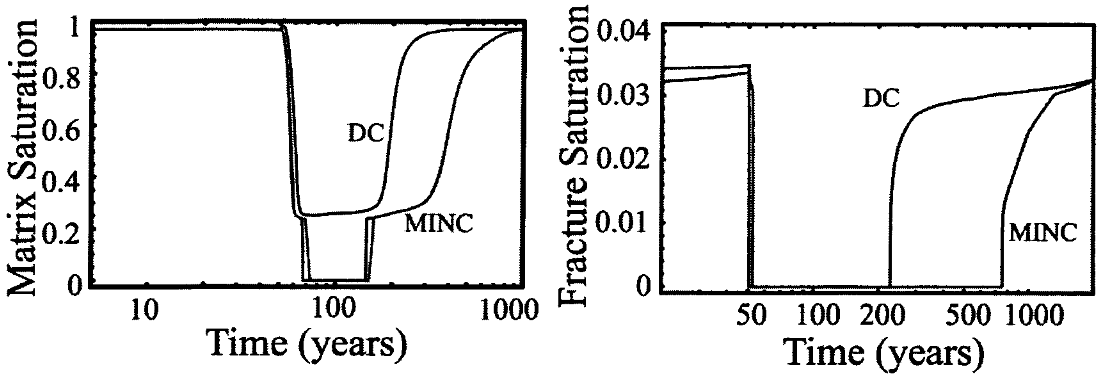

Figure 4: Matrix and fracture saturations at the tunnel crown versus time for dual continua (DC) and MINC representations. The heat load into the rock is reduced by 75% during the first 50 years in this case.

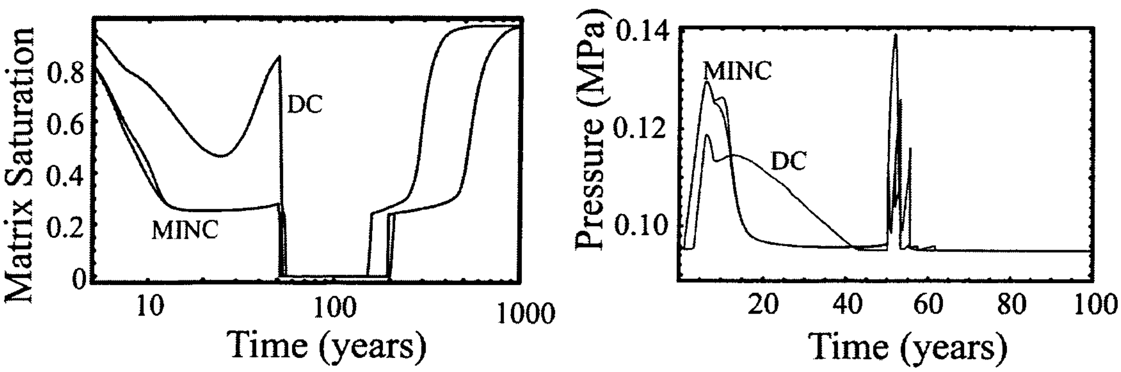

Figure 5: Matrix saturation and pressure at the tunnel crown versus time for dual continua (DC) and MINC representations. The heat load into the rock is reduced by 50% during the first 50 years in this case.