Project 00087003 - Advanced Conceptual Models for Unsaturated and Two-Phase Flow in Fractured Rock

Final Report for University of Colorado Portion of the Project

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Research Objective: The Department of Energy Environmental Management Program is faced with two major issues involving two-phase flow in fractured rock; specifically, transport of dissolved contaminants in the Vadose Zone, and the fate of Dense Nonaqueous Phase Liquids (DNAPLs) below the water table. Conceptual models currently used to address these problems do not correctly include the influence of the fractures, thus leading to erroneous predictions. Recent work has shown that it is crucial to understand the topology, or 'structure' of the fluid phases (air/water or water/DNAPL) within the subsurface. It has also been shown that even under steady boundary conditions, the influence of fractures can lead to complex and dynamic phase structure that controls system behavior, with or without the presence of a porous rock matrix. Complicated phase structures within the fracture network can facilitate rapid transport, and lead to a sparsely populated and widespread distribution of concentrated contaminants; these qualities are highly difficult to describe with current conceptual models. The focus of our work is to improve predictive modeling through the development of advanced conceptual models for two-phase flow in fractured rock.

Research Approach:

For fluid invasion, preliminary experiments have shown that behavior at fracture intersections is key, thus we are employed systematic experimentation to identify and classify behavior at intersections. The role of fracture intersections as integrators in the case of wetting fluid infiltration has also been vividly demonstrated. This leads to a new class of conceptual models for infiltration in fractured vadose zones, based on concepts from self-organized criticality. These models predict interesting types of episodic infiltration events at several scales, and may explain field observations that exhibit spatio-temporal complexity including episodic behavior. In the case of non-wetting fluids, intersections are readily invaded and fingers emanate from invaded intersections, with little temporal fluctuations.

Understanding gained at the scale of individual fracture intersections was used to augment a Modified Invasion Percolation Model (MIP) that has shown significant promise in predicting flow through fracture networks. The augmented, and fully tested MIP model was exercised on realistic fracture networks for the purpose of understanding large-scale development of phase structure. The fracture networks were generated based on recently published synthesis of observations at many well-studied sites. The implications of complex phase structure and fracture network topology on transport processes was also investigated based on detailed numerical simulations.

Progress in Previous Years: Progress in previous years was reported in the mid-term report submitted previously and has led to eighteen journal publications overall.

Summary of Research Accomplished at University of Colorado:

The Modified Invasion Percolation (MIP) model was augmented to explicitly represent intersections, and implement rules at fracture intersections to mimic capillary barrier type behavior in the case of a wetting fluid. Simulations on an experimental network (Glass et al., Water Resources Research, 2003) compared favorably with experimental observations, specifically demonstrating the formation of a slender-ladder type wetted phase structure. A set of computer codes were developed for generation of fracture networks, and definition of variable-aperture fields within individual fractures and at fracture intersections, for purposes of invasion simulations. A series of simulations were carried out on computer-generated fracture networks with power-law length distributions. The results of these simulations demonstrate a tendency for slender phase structures to form even in rather complex and dense fracture networks, aided by gravitational forces. Simulations of the invasion of a dense non-wetting phase liquid were also carried out, illustrating differences in behavior at an intersection. An example of an inclined slender ladder structure for a wetting phase invasion into a fracture network is shown in Figure 1. The enhanced MIP algorithm was applied to a quasi three-dimensional fracture network (in the sense that the network itself has a two-dimensional topology, while a third dimension is added by extruding the network), with variable apertures. The fracture traces were generated using a power-law length distribution (the probability density function for fracture length is of the form $p(l) \sim l^{-a}$, for $l_{min}<l<l_{max}$), with random positioning of fracture centers and an orientation distribution with 80% probability of an orientation at 30 degrees to horizontal and 20% probability of being oriented at 85 degrees to the horizontal. A recent review paper (Bonnet et al., 2001) discusses the relevance of power-law length distributions to natural fracture networks extensively. The upper and lower bounds for fracture lengths were set at 0.5 and 0.1 times the domain size respectively, in the simulation shown. The number of fractures in the network is 174 and there is a percolating path from the top to the bottom of the network through the fractures. The mean aperture in a fracture was correlated to fracture length according to the relationship aperture ~ $\text{length}^{0.5}$, which is similar to relationships discussed in the review article of Bonnet et al. (2001). This correlation systematically leads to larger apertures in longer fractures. A constant value of the coefficient of variation = 0.1 (standard deviation/mean) was used in all fractures to represent aperture variability within the fracture plane. An example of a complex DNAPL pool generated by invasion of a dense non-wetting liquid is shown in Figure 2.

In the broad context of two-phase flow in fractured rock, the role of vapor-phase transport is important in the context of drying either in the vicinity of ventilated drifts, or due to topographically/barometrically induced air flow through fractures, as has been documented at several sites, including Yucca Mountain. Vapor phase transport by drying in single fractures and fractured rock masses were investigated both experimentally and computationally. The experimental studies were performed using time-domain reflectometry (TDR) measurements of water contents in rock masses adjacent to ventilated fractures. The conventional TDR measurement system needed to be modified to apply to rocks, requiring special attention to gap effects and development of rock-specific calibration functions. We showed that simple surface probes and penetration-type probes with the use of conductive silicone as a gap filler are capable of accurate water content measurements in rocks. We developed a new approach for coupling vapor transport in fractures and the rock matrix using the Kelvin equation at the interface, thus allowing the use of a simple nonlinear diffusion equation for moisture diffusion in the rock matrix coupled to the advection-diffusion equation for vapor in the fracture. This approach was also applied to fracture networks, and led to interesting insights in the influence of network structure on bulk drying rates (Figure 3) induced by ventilation of fractures.

Solute transport within a variable-aperture fracture with an entrapped non-wetting phase was investigated, specifically to evaluate the role of the entrapped phase on solute transport behavior. We identified an important type of scale-invariance that may be expected in solute transport through two-phase flows in variable fractures: The entrapped phase geometry exhibits scale-invariant properties, because it results from a modified percolation-type invasion process. In other words, the size distribution of entrapped blobs scale with domain size (fracture size) rather than the correlation length of the aperture field, so that significant non—Fickian features may be expected in solute transport in any fracture under two-phase flow conditions (Figure 4). However, development of a suitable theoretical model for transport in these types of flows remains elusive, a single transport model does not adequately capture the behavior seen across the full range of entrapped phase geometries.

Information Access: Publications Resulting From University of Colorado Portion of Research Project

Glass, R.J., M.J. Nicholl, H. Rajaram, and T.R. Wood, Unsaturated flow through fracture networks: Evolution of liquid phase structure, dynamics, and the critical importance of fracture intersections, Water Resources Research, Vol. 39, (12) No. 1352 doi:10.1029/2003WR002015, 2003.

Glass, R.J., M.J. Nicholl, H. Rajaram, and B. Andre, Development of slender transport pathways in unsaturated fractured rock: Simulation with Modified Invasion Percolation, Geophysical Research Letters, 31, L06502, doi:10.1029/2003GL019252, 2004.
Holt, R.M. and M.J. Nicholl, Uncertainty in vadose zone flow and transport prediction, Vadose Zone Journal, 3, 580-584, 2004.

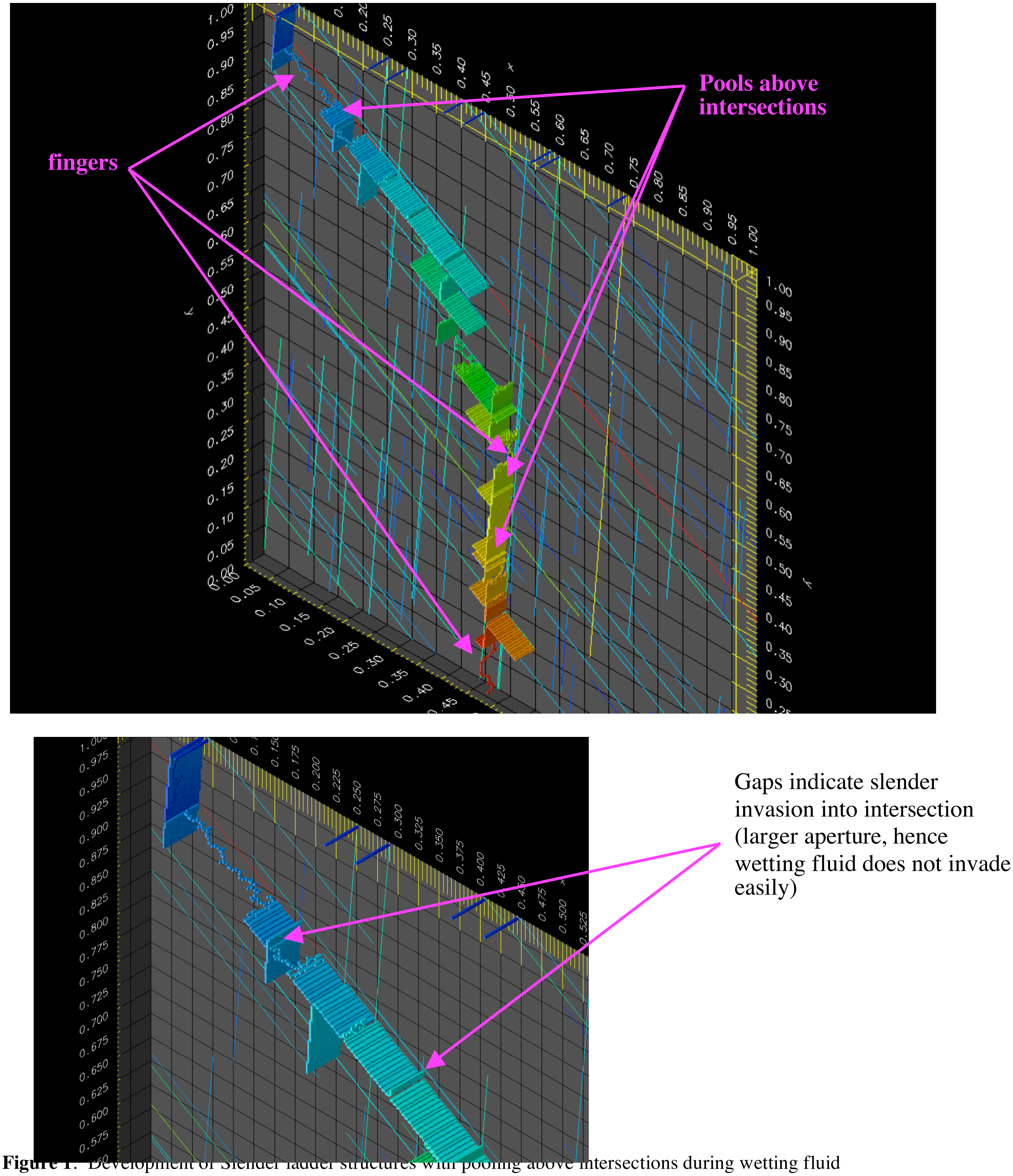
Molz, F.J., H. Rajaram, and S. Lu, Stochastic fractal-based models of heterogeneity in subsurface hydrology: Origins, applications, limitations and future research questions, Reviews of Geophysics 42, RG1002, Paper No. 2003RG000126, 42 pages, 2004.

Sakaki, T., and H. Rajaram, Performance of different types of TDR probes for water content measurement in partially saturated rocks, Water Resources Research, 42, W07404, doi: 10.1029/2005WR004643, 2006.

Sakaki, T., 2005, The role of fracture-matrix interaction in drying of unsaturated fractured rock, Ph.D. thesis, University of Colorado.

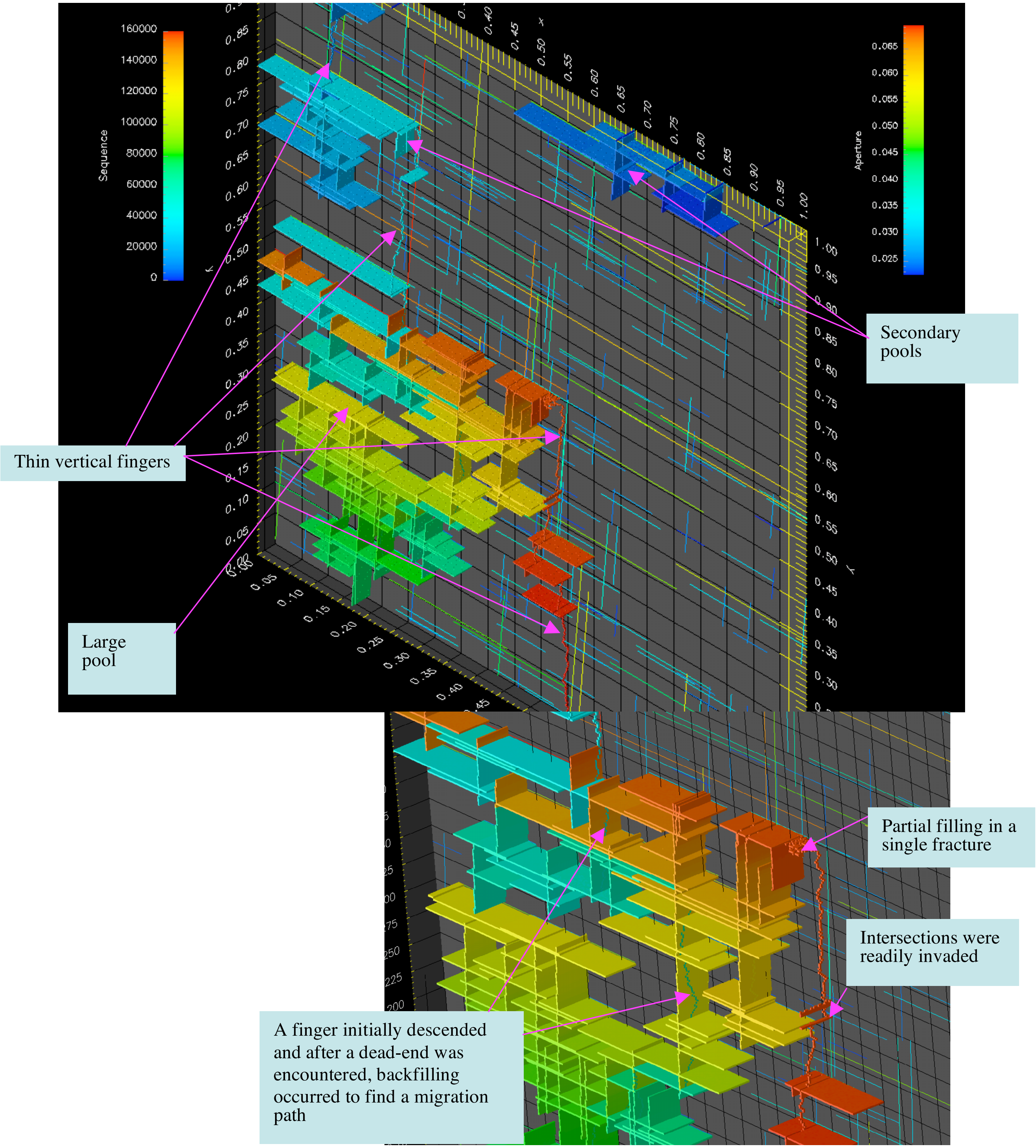
Bliss, Matthew, J., 2005, Solute transport in partially saturated variable-aperture fractures, M.S. thesis, University of Colorado.

Other publications are in preparation.



Gaps indicate slender invasion into intersection (larger aperture, hence wetting fluid does not invade easily)

Figure 1: Development of Slender ladder structures with pooling above intersections during wetting fluid invasion in a fracture network. The colors for water invaded regions indicate the sequence of invasion (Dark blue -> light blue -> green -> yellow -> red represents early -> late invasion). The color scale for fracture apertures (traces shown against back of domain) is used to represent fracture apertures (red for large apertures -> dark blue for small apertures)



Secondary pools

Thin vertical fingers

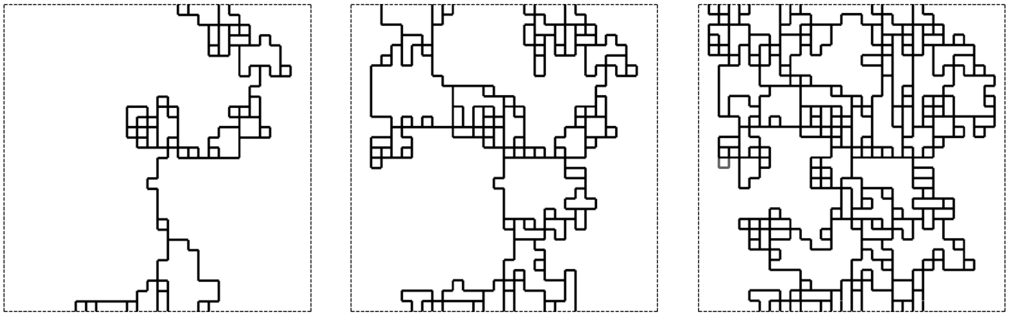
Large pool

Partial filling in a single fracture

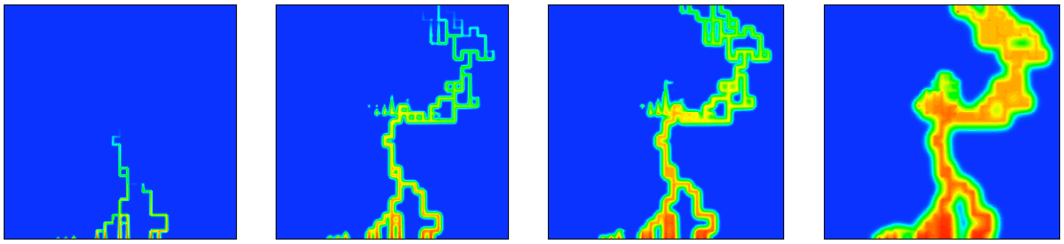
Intersections were readily invaded

A finger initially descended and after a dead-end was encountered, backfilling occurred to find a migration path

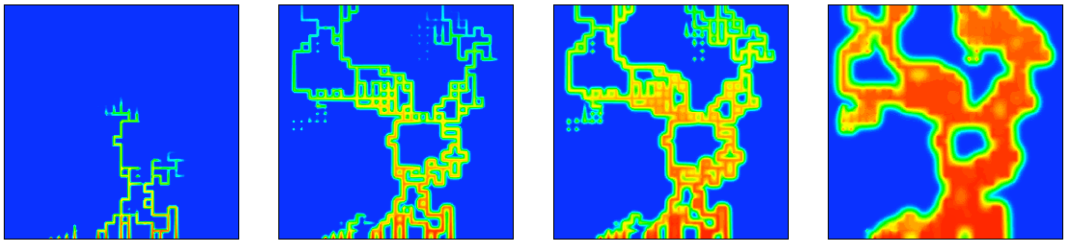
Figure 2: Results of a TCE migration simulation in a quasi-three-dimensional fracture network and an enlarged region of the resulting TCE source zone. TCE invaded the water-saturated medium from the top, and the colors for TCE invaded regions indicate the sequence of invasion (Dark blue -> light blue -> green -> yellow -> red represents early -> late invasion). The color scale for fracture apertures (traces shown against back of domain) is used to represent fracture apertures (red for large apertures -> dark blue for small apertures). The resulting source zone exhibits pooled regions of TCE separated by narrow fingers where displacements became unstable in vertical fractures. Also observed in this simulation is preferential invasion of fracture intersections and partial filling of horizontal fractures due to the influence of capillarity. The complex distribution of TCE in this relatively simple fracture network clearly illustrates the difficulties with representing TCE source zones in fracture media using a continuum approach.



(a) $p = 0.52$



(b) $p = 0.55$



(c) $p = 0.60$

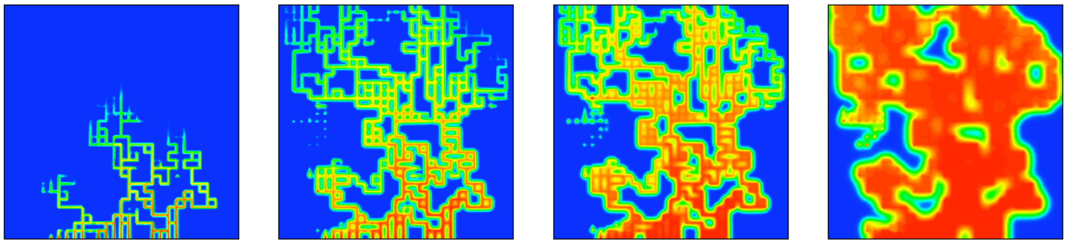


Figure 3: (from Sakaki, 2005, thesis) Illustration of the influence of network connectivity in percolation networks (p is the probability that a bond is not removed, starting from an initially complete network). The images show drying (by nonlinear moisture diffusion) of a rock mass by fracture ventilation. Dramatic variations in "effective diffusivity" can result from flow-weighted effective surface area and network connectivity.. The color scale represented moisture content, with blue=wet and red=very dry. For each value of p, the sequence from left to right shows the evolution of moisture content over time.

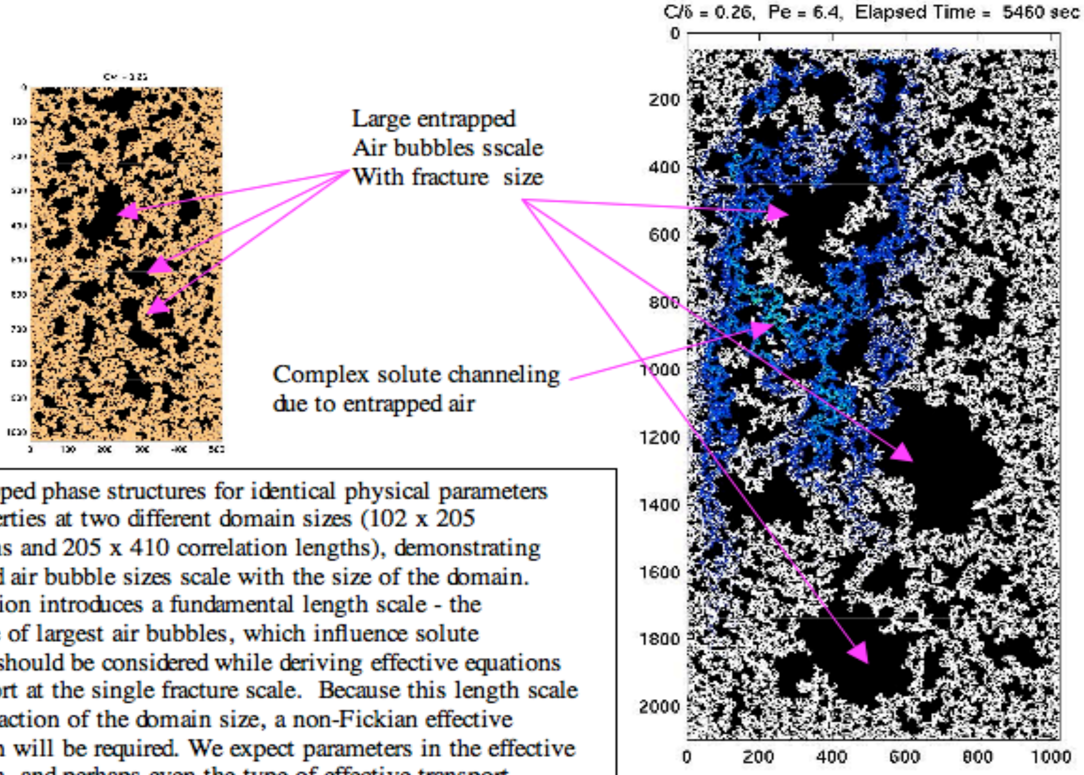


Figure 4

Entrapped phase structures for identical physical parameters and fracture properties at two different domain sizes (102 x 205 correlation lengths and 205 x 410 correlation lengths), demonstrating that the entrapped air bubble sizes scale with the size of the domain. Invasion percolation introduces a fundamental length scale - the characteristic size of largest air bubbles, which influence solute channeling, that should be considered while deriving effective equations for solute transport at the single fracture scale. Because this length scale is a significant fraction of the domain size, a non-Fickian effective transport equation will be required. We expect parameters in the effective transport equation, and perhaps even the type of effective transport equation to vary as the wetting phase saturation varies. Note that the above phase structures and the wetting phase saturations shown in the graph correspond to capillary-dominated invasions (e.g. horizontal fractures). When gravity effects are included, fingered phase structures (low wetting phase saturations) will result, with completely different transport behavior. Thus transport parameters will not depend only on wetting phase saturation, additional parameters such as the Bond number will influence phase geometry and hence transport parameters.