

## A PARTICLE-TRACKING APPROACH TO MODELING TRANSPORT IN A COMPLEX FRACTURE

Chin-Fu Tsang and Christine Doughty

Contact: Christine Doughty, 510/486-6453, cadoughty@lbl.gov

### RESEARCH OBJECTIVES

Nearly all of the studies of flow and transport in fractured rocks assume that a fracture can be modeled as an open space between two rock surfaces with constant or variable separation. Field observations of rock fractures have shown that a fracture in the field can in fact be much more complex. Recent studies indicate that a complex fracture can be characterized as a thin fracture zone having several interconnected subfractures (Figure 1), which can contain mechanically dislodged and chemically altered materials with enhanced porosity. Our objective is to develop a model for flow and transport through a fracture that incorporates these complexities.

### APPROACH

We use a particle-tracking approach to calculate solute transport in a complex fracture, accounting for transmissivity variability over the fracture plane, and incorporating structures in the fracture thickness normal to the fracture plane. These structures include subfractures, dead-end pores, gouge materials, small blocks of altered rock, and the adjacent "semi-infinite" rock matrix. The subfractures provide alternative flow paths for advection, whereas the remaining features all provide material in which solute diffusion and sorption can occur (Figure 1). Flow through the fracture plane is calculated numerically using a finite-difference method, and advective transport is modeled with particle tracking. For each particle, flow is distributed among the subfractures; then, for each gridblock, a time delay is added to the advective residence time to account for diffusion and sorption into adjacent lower-permeability materials. The time delay for each particle is obtained stochastically, by inverting an analytical solution for diffusion and sorption into finite-sized matrix blocks.

### ACCOMPLISHMENTS

The above approach has been applied to a field study of a single complex fracture on the 15 m scale. Fracture mapping and pump-test results were used to characterize the transmissivity distribution within the fracture plane. Tracer tests using sorbing and nonsorbing tracers were analyzed to infer the near-fracture parameters of the complex fracture model, including distribution of flow between subfractures as well as diffusion and sorption into gouge and intermediate matrix blocks. Short-term tracer tests are less sensitive to properties of the semi-infinite rock matrix, so laboratory analyses of unaltered rock samples should

be used to obtain those properties. When considering time scales of thousands of years, as needed for nuclear waste storage per-

formance assessment, properties of the semi-infinite matrix have a much more significant role. Results show that the proposed method is feasible, efficient, and can match field tracer-test data. Additionally, the parameter dependence and sensitivity are reasonable for both short-term (site characterization) and long-term (performance assessment) studies.

### SIGNIFICANCE OF FINDINGS

If a simple fracture model, based on the conventional advective-dispersive equation, is used to match the tracer breakthrough curves obtained from a complex fracture, serious problems arise. In the simple fracture model, multiple flow paths within the fracture and diffusion and sorption into gouge materials and intermediate

blocks are ignored, and thus their effects have to be represented by the property values of the semi-infinite rock matrix. This leads to calibrated values significantly larger than laboratory measurements of the rock matrix samples, which in turn leads to significant errors in long-term (performance assessment) models. This may be one significant source of the so-called scaling effect.

### RELATED PUBLICATIONS

- Tsang, C.-F., and C. Doughty, A particle-tracking approach to simulating transport in a complex fracture. *Water Resour. Res.*, 39(7), 1174, doi:10.1029/2002WR001614, 2003. Berkeley Lab Report LBNL-50537.
- Doughty, C., and M. Uchida, PA calculations for feature A with third-dimension structure based on tracer test calibration. IPR-04-33, Swedish Nuclear Fuel and Waste Management Co. (SKB), Stockholm, Sweden, 2003.

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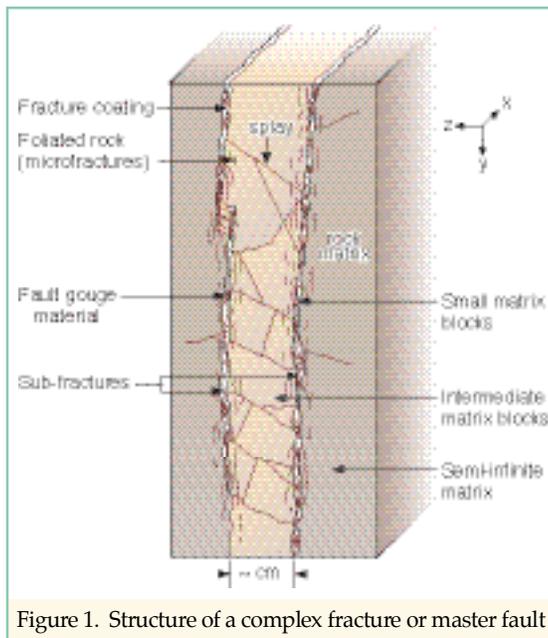


Figure 1. Structure of a complex fracture or master fault

