Scale-Dependent Fracture-Matrix Interactions And Their Impact on Radionuclide Transport

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Abstract: Matrix Diffusion and Adsorption within a rock matrix are important mechanisms for retarding transport of radionuclides in fractured rock. Due to computational limitations and difficulties in characterizing complex subsurface systems, diffusive exchange between a fracture network and surrounding rock matrix is often modeled using simplified conceptual representations. There is significant uncertainty in "effective" parameters used in these models, such as the "effective matrix diffusivity". Often, these parameters are estimated by fitting sparse breakthrough data, and estimated values fall outside meaningful ranges (e.g. effective matrix diffusivity much greater than free molecular diffusivity), because simplified interpretive models do not consider complex three-dimensional flow. There is also evidence for an apparent scale-dependence in effective matrix diffusivity, also a consequence of using over-simplified interpretive models. These observations raise questions on whether fracture-matrix interaction parameters estimated from small-scale tracer tests can be used for predicting radionuclide fate and transport at the scale of DOE field sites.

High-resolution three-dimensional Discrete-Fracture-Network-Matrix (DFNM) models based on well-defined local scale transport equations can help to address some of these questions. Due to tremendous advances in computational technology over the last 10 years, DFNM modeling in relatively large domains is now feasible. The overarching objective of our research is to use DFNM modeling to improve fundamental understanding of how effective parameters in conceptual models are related to fracture network structure and matrix properties. An advanced three-dimensional DFNM model is being developed, which combines upscaled particle-tracking algorithms for fracture-matrix interaction and a parallel fracture-network flow simulator. The particle-tracking algorithms allow complexity in flow fields at different scales, and track transport across fracture-matrix interfaces based on rigorous local approximations to the transport equations. This modeling approach can incorporate aperture variability, multi-scale preferential flow and matrix heterogeneity. The code can handle computational domains with about 1 Billion nodes for flow and 1 Billion particles for transport. The overarching goal is to obtain insights on (i) the relationship between effective fracture-matrix interaction parameters, network structure and matrix properties and (ii) their scale dependence in different types of fractured rock environments.

We will demonstrate results obtained using "high-resolution" particle tracking algorithms at the single fracture scale and at fracture intersections; and "upscaled" particle-tracking algorithms, which allow use of much larger time steps. The upscaled algorithms have been verified using the "very-high-resolution" simulation results as a benchmark, and hold significant promise as an efficient tool for field-scale simulation. A generalized approach for particle tracking in interfaces has been developed, which captures the complexities of Stokes flow through variable-aperture intersections with excellent accuracy. Flow simulations in fracture networks illustrate the important role of head variations along an intersection in driving flow through slow advective loops in dead-end fractures. Such loops have been postulated as potential mechanisms for producing long-tailed behavior even in the absence of true matrix diffusion, and often confused for matrix diffusion. Ongoing efforts are focused on extending the network flow and transport simulations to very large scales, and including the influence of adsorption.

The final stage of our research will specifically target applications at the Oak Ridge Field Research Center, former nuclear test sites in Nevada (e.g. the Shoal and Bullion tests), and other field sites (e.g. Mirror Lake) where tracer tests were conducted to obtain fracture-matrix interaction parameters for site-scale transport models. We will explain the differences in behavior observed at these sites using our network model and subsequently simulate radionuclide transport at the site scale and 100+ year time scales.