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Effects of cross-scale fracture surface roughness in crystalline host rocks on hydrodynamics

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Granite is considered a suitable host rock for a deep geological repository for radioactive waste. Since fractures are the main flow pathways for solute transport in this material, accurate and efficient calculation of solute transport and retention phenomena is essential for predictions related to the safety case of the repository. A key issue is the effect of cross-scale surface topography and roughness on hydrodynamics such as fluid channeling and residence time. In this study, we use a fracture geometry model based on μ-CT data and apply a finite element method to reveal the influence of fracture geometry on solute transport behavior. Due to the heterogeneity of fracture shape and aperture width distribution, it is difficult to describe the fracture geometry and morphology by a single variable. In addition, the surface roughness of fracture walls exhibits cross-scale variability due to heterogeneous material composition, which hinders the application of simplifying self-affine geometry descriptions. Instead, investigating of the role of cross-scale surface roughness in solute transport modeling is a promising approach. We investigated the sensitivity of the roughness effect by systematic modification across scales using μ-CT data of granite fractures. By comparing 2.5D vs. 3D transport model results, the role of long wavelength surface constituents and fracture bending can be investigated. The solute transport modeling was performed using the finite element code COMSOL Multiphysics. We discuss the quantitative effect of long wavelength surface building blocks on the tailing of the breakthrough curves and a weakening of the Fickian behavior. The tracer concentration fields in the 2.5D models show a high sensitivity to spatial heterogeneity. The solute transport in larger half-pores is overestimated compared to 3D models. The differences between 2.5D and 3D models due to small-scale surface roughness are considerably smaller. Nevertheless, the effect of surface roughness wavelengths on the BTC tailing behavior is not simply monotonic, which is an important effect to consider when implementing roughness parameters in transport modeling. Finally, we discuss the potential application of using power spectral density (PSD) curves as a means of assessing changes in roughness on fracture surfaces. PSD curves provide a cross-scale quantification of surface topographies. We propose the implementation of PSD curves in transport models to increase their predictive capability for contaminant migration in fractures.

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References

Primary author: Mr ZHOU, Wenyu (HZDR, FS Leipzig)

Co-author: FISCHER, Cornelius (HZDR, FS Leipzig)

Presenter: Mr ZHOU, Wenyu (HZDR, FS Leipzig)

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