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Improved predictability of numerical flow models of fractured crystalline media: The effect of surface roughness.

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Transport and flow through fractured crystalline rocks is an important and often studied topic in the context of nuclear waste disposal, given that the heterogeneity of fluid transport constraints the efficiency of radionuclide sorption processes. In past years, several studies have provided numerical simulations of the flow rate that can be expected in different types of fractures. Such studies rely on the required length-scale and spatial resolution of geometrical data in order to conduct flow and transport modeling. The numerical results are validated against tracer data of break-through experiments, such as the recently available spatiotemporal tracer concentration analysis, obtained from positron emission tomography (PET) . In many cases, however, the results obtained from the numerical simulations differ greatly from the experimental observations. While some numerical models commonly operate under the cubic law assumption, which defines a fracture as two perfectly parallel smooth surfaces, more advanced simulations include the effect of fracture surface roughness. Such results suggest the need of an improved understanding of transport heterogeneities as a function of fracture surface roughness and topography. Moreover, a systematic evaluation provides insight into the model complexity required for reliable radionuclide transport and flow predictability in potential host rocks.

In this study, we focus on the numerical modeling of flow through a fracture while taking into account surface roughness of the fracture walls, and validating the results against tomographic methods. For this purpose, the structural parametrization of the fracture is carried out by performing the segmentation of micro-computed tomography (μCT) images obtained from Granite samples from the Mrákotín quarry in the Czech Republic. Subsequently, interferometry measurements of identical fracture material are carried out in order to quantify the details in the surface topography at the nm to μm scale. Resulting data are combined with μCT data through statistical methods, which provide a more meaningful definition of the surface topography, and are compared with numerically generated surface roughness. Resulting numerical simulations are then validated against PET measurements. As a result from the outlined workflow and the quantitative comparison, we provide suggestions of general applicability of the required degree of complexity for surface geometry segmentation in flow simulations.