On the relevance of discontinuities and geochemical heterogeneity in the reactive transport behavior in fractured rocks

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Understanding of groundwater flow and solute transport in discrete fracture networks (DFN) is crucial to assess the safety of deep geological repositories for nuclear waste in crystalline rocks. It is well known that groundwater flow in such environments is controlled by discontinuities, and that traditional continuous porous media theory, based on defining a Representative Elementary Volume does not apply in most cases. However, to simulate the hydrogeological behaviour of such DFN descriptions may lead to unpractical and expensive computational costs. This is the main reason why large research efforts have been devoted to test and developing different methodologies for upscaling from DFN representations to Equivalent Continuous Porous Media approach (ECPM). Successful results in terms of groundwater flow have been achieved in the last decades, but still very limited applicability when solute transport and geochemical processes are considered. In this work, we will show numerical methodologies for solving solute transport and geochemical processes in DFN, and some ideas about future trends for upscaling transport and geochemical properties.

On the other hand, mineral surfaces and pore space in rock are distributed in complex microstructures and their distributions are far from being homogeneous. Such heterogeneities occur at the submillimetre scale and are usually ignored by larger scale traditional reactive transport models based on averaged geochemical parameters. In this work, we use High Performance Computing technology to assess the implications of grain-scale physical and mineralogical heterogeneity on the macroscopic transport and geochemical behaviour of radionuclides. The resulting grain-scale reactive transport models are solved in a supercomputer, and the results are compared with macroscopic upscaled models, where mineral abundance is averaged over the matrix volume.

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