Surface reactivity and transport concepts: Lessons learned from submillimetre reactive transport modelling

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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. In the grain-scale model, the penetration of radionuclides into the rock is faster and the penetration front is uneven and finger-shaped. The analysis of computed results shows that the upscaled macroscopic (traditional) continuum-scale models provide later first-arrival time estimates compared to the grain-scale model. We also show the concept of grain-scale Inter-Granular Network model (IGN), and how it has been used to offer plausible explanations for apparently anomalous radionuclide penetration profiles observed in some in-situ and laboratory experiments.