



Coupled dissolution-precipitation reactive transport modeling at the pore scale

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Coupled dissolution-precipitation processes are of critical importance for the evolution of porosity and permeability in materials and for multiple applications, such as waste management, reservoir rocks, and corrosion. Here, we study the impact of saturation and fluid flow velocity with high spatial resolution, i.e. in the micrometer to submicrometer scale. Utilizing a time series of datasets of corroded crystal surfaces, collected using interferometry techniques, we analyze the impact of local fluid flow heterogeneity and resulting saturation variability. Systematically, the series of surface data is used (i) to constrain the initial topography for reactive transport modeling, and (ii) to compare the model vs. experimental results.

In this work, a reactive transport model is presented which simulates the complex chemical reaction of mineral dissolution/precipitation and subsequent pore-geometry evolution at a single pore scale [1]. We used the finite element package COMSOL Multiphysics[®] 5.4 for the simulation, utilizing the arbitrary-Lagrangian Eulerian (ALE) method for the free-moving domain boundary.

Experimental and modeling studies have shown both the spatial [2] and temporal [3] heterogeneity of reaction rates and their impact on topography evolution at the pore scale. We expect an improved predictability of reactive transport modeling by using an approach combining the heterogeneities of surface reactivity and flow velocity at the pore scale.

[1] Karimzadeh, L., et al., 2018. Benchmark 3D reactive transport modelling of leaching of fractured calcareous sulfide ores, in: Lottermoser, B.G. (Ed.), Aachen International Mining Symposia (AIMS 2018), Aachen, Germany, p. 88

[2] Fischer, C., and Luttge, A., 2018, Pulsating dissolution of crystalline matter. PNAS 115, 897.

[3] Fischer, C., Kurganskaya, I., and Luttge, A., 2018, Inherited control of crystal surface reactivity. Applied Geochemistry 91, 140.