Dynamic simulation of diffusion controlled celestite precipitation in a µCT-generated pore space

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We present a novel and promising idea of a reactive fluid dynamics modelling approach verified by data of a previously described mineral precipitation experiment [1]. In our experimental setup, both ends of a compacted and water-saturated sand column were each connected to a reservoir containing either $SrCl_2$ or Na_2SO_4 solution at equal concentrations. A sharp precipitation front of less soluble celestite ($SrSO_4$) developed in mid of the sand column under counter-diffusion controlled conditions, but did not clogg the pore space even after 4 weeks. Computed micro-tomography (µCT) imaging was used before and after the precipitation reaction to quantify the thus changed porosity and permeability. Our model workflow used the µCT-generated (real) pore space geometry as input and coupled a robust solver for diffusive particle transport with a geochemical calculator. The GeoDict software package (Math2Market, Germany) was used to simulate particle diffusion paths applying its AddiDict module. The virtual nanoparticles generated in AddiDict (100,000 at each end of column) were set at a limited volume (minimum one order of magnitude smaller than µCT voxel size), which was filled up with the counter-diffusing solutes. The two virtual solute particle swarms in the saturated pore space represent thereby the counter-diffusing solutes chemistry. The geochemical equilibrium code PHREEQC (USGS, v3) was coupled to simulate the probability of pore cement precipitation wherever it can be expected on basis of an appropriate SI developing once individual solute particles hit each other in the pore space. In our workflow, MATLAB (MathWorks, v2013a) scripts automatically access GeoDict control data files, and Python scripts (Python Software Foundation, v2.6.6) embed both the transport and geochemistry codes into a time loop for sequential simulation of pore-scale reaction and transport parameters. First simulation runs on a MPI-HPC platform successfully reproduce the experimental development, shape and thickness of the precipitation front as well as the concomitantly changing HTO tracer transport.

[1] Chagneau et al. (2015) *Geochem. Transactions* **16**, 1-13.