Pore-scale simulation of calcite cement dissolution in sandstone

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We present a new reactive transport modeling approach coupling heterogeneous flow physics and calcite mineral dissolution at pore scale resolution. A model workflow coupling different numerical solvers has been developed according to the operator splitting method involving a Lagrangian particle transport approach. The FlowDict module of the GUI-based GeoDict software package (https://www.math2market.com/Modules/Dicts/FlowDict.php) iteratively computes the local permeability and flow field of a given three-dimensional porous geometry by applying the Navier Stokes Brinkman equations. The LIR-tree algorithm serves as a framework for enhancing numerical efficiency by partitioning the computational domain [1]. The domain size is usually 1024^3 voxlels of 0.74 μm edge length. Each voxel consists of a void, calcite cement or inert quartz matrix. The AddiDict module simulates the advective and diffusive motion of myriads of virtual nanoparticles much smaller than voxel size. These particles carry aqueous solutions into the pore voxels, which admix to the pore fluid solutions and/ or react once bouncing at surfaces resulting in local surface dissolution or precipitation of the solid mineral phase at the sub-voxel scale. Kinetically controlled geochemical reactions are implemented by the C++ library of the open-source code Phreeqc-RM (USGS). Multiple MPI-processes and OpenMP threads are applied to provide upon parallelization for an efficient HPC performance of the C++ code. Our code framework enables to embed all mentioned modules into a time loop for sequential time-lapse simulations of the processes. In our benchmark study, the microstructure was imported directly from synchrotron-based computed tomography data. An inflowing acidic solution particles front invades increasingly the locally equilibriated pore fluid ultimately triggering dissolution reactions at calcite cement surfaces. Local pressure, permeability and velocity are thus considered not only to vary in space but also in time. Our results (time-lapse movies) show the effects of local pore space alterations on dynamics of fluid and solutes (e.g., pH and Ca concentrations) calculated according to our novel Digital Rock Physics concept.

[1] Linden, Wiegmann & Hagen (2015) *Graph. Models* **82**, 58–66.