# Dynamic simulation of kinetic calcite dissolution in a µCT-generated pore space

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We present a novel and promising idea of a reactive fluid dynamics modelling approach at pore scale resolution. A model workflow combining numerical solvers has been developed according to the operator splitting approach and the Lagrangian transport method. The FlowDict module of the GeoDict software package (Math2Market GmbH, Germany) iteratively computes the flow field of a given three dimensional porous geometry by applying the Navier Stokes-Brinkman equation. The AddiDict module (Math2Market GmbH) simulates the advective and diffusive motion of virtual particles. These particles carry aqueous solutions, which mix with pore fluid solutions and react once bouncing at surfaces resulting in dissolution and/or precipitation of mineral phases at the sub-voxel scale. Kinetically controlled geochemical equilibrium calculations are performed by the C++ library of the open-source code PHREEQC (USGS). Our code embeds the prior mentioned modules into a time loop for sequentially simulating pore-scale reactive transport at changing solid matrix volume. GeoDict control and data files are automatically accessed to communicate the processed geochemical data. Multiple MPI-processes are applied to provide an efficient performance of the C++ Lagrangian reactive transport code.

Results show effects of local pore space alterations on the continuously changing hydromechanical transport parameters calculated according to the Digital Rock Physics concept. Kinetic calcite dissolution has been simulated in a µCT structure, whereby an inflowing pure water solution mixes with a calcite equilibrium pore fluid solution triggering dissolution reactions at calcite surfaces (Fig. 1).

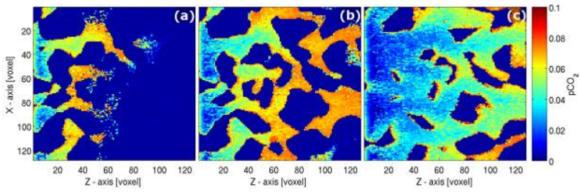

**Fig. 1:** Representative 2D slices (a-c) of proceeding time steps show the calcite grain dissolution visualized as increasing $pCO_2$ values in the pore matrix. Inflow is from left to right.