A microfluidic experiment and pore scale modelling for assessing mineral precipitation and dissolution in confined spaces

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The precipitation and dissolution of minerals in porous media are important processes in geological and technical settings. Such reactions can alter the porosity, permeability, and other physical characteristics of the rock matrix that can affect solute transport. In order to bridge atomistic and macroscopic scales, it is necessary to understand the processes and subsequently to upscale the pore-scale results to macroscopic simulation codes. In this direction, we developed a methodology combining a sophisticated microfluidic experimental setup and cross-scale modelling numerical diagnostics. This allows exploring the processes of mass transport coupled to nucleation, mineral precipitation and dissolution in confined spaces. A system with relatively few chemical species, but with well-defined kinetic parameters was chosen to establish a "proof of concept". The pore scale modelling of the processes inside the microfluidic reactor was based on the Lattice Boltzmann method and was used to spatially resolve the solution composition not accessible experimentally, to calculate the local saturation indices using full speciation, and to predict the induction time for the nucleation process. The information gained from the cross-scale pore-level model helped to gain insights into the underlying precipitation mechanisms and to explain the preferential growth direction of the crystals during the experiment.