



Effects of nucleation on mineral dissolution and precipitation predicted from reactive pore scale simulations

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Reactive rate constants are usually determined experimentally by using well-stirred batch reactors where the mass transfer from the mineral phases to the aqueous solution is monitored continuously. The reactive rates observed in flow through core scale experiments can differ by several orders of magnitude compared to well-stirred reactors. Multiple factors contribute to the difference: real rock minerals are not pure minerals due to incorporated trace elements; the reactive surface area of the individual mineral phases in a rock is usually unknown; multiple minerals are present at the same time, and the overall rate is usually governed by the slowest process; secondary minerals precipitate and partly cover the primary minerals.

In this work, we present pore scale reactive flow simulations that investigate the effect of nucleation, precipitation and dissolution on permeability, surface area, and the effective reaction rates in chalk samples obtained from different types of outcrop chalk. The pore geometries are composed of segmented FIB-SEM images of real chalk samples. The injection of magnesium-chloride ($MgCl_2$) in these samples leads to calcite dissolution and magnesite precipitation. In our model, all the surface area is available for dissolution, but precipitation is only possible at certain nucleation sites. Our nucleation model is not based on e.g. the local specie concentration or the surface topology. Instead, we randomly prescribe a given fraction of the solid nodes to act as nucleation sites. Nucleation is often not included in reactive flow simulations, but our results demonstrate that variations in nucleation has a significant effect on the pore scale properties. Hence, pore scale simulations need to incorporate some form of nucleation model when used to interpret mineralogical alterations observed in flooding experiments.

The numerical model uses lattice-Boltzmann (LB) to solve the advection-diffusion equation for the species and pore fluid, and a geo-chemical solver to calculate the mass-flux across the solid-fluid interface caused by dissolution and precipitation processes using a non-linear rate-law with kinetic rate constants specific to each mineral phase.