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Reactive flow simulations: one-to-one comparison with experiments

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Direct in-situ observations of structural changes in the pore space of porous rocks during reactive flow provide valuable insights into the pore scale mechanisms that govern mineral growth, changes in wetting properties and increased oil recovery. We present simulations of single-phase reactive flow in micrometer sized channels in a calcite (CaCO₃) crystal and compare mineralogical and geometrical changes in the numerical results to experimental in-situ observations made with the same flow geometry and reactive fluids. This enables a rigorous test of the numerical model and a method for determining kinetic rate constants that will be used in simulations of reactive flow in chalk geometries. The numerical model is a lattice Boltzmann model (LBM) that moves a set of chemical basis species through the pore space by advection and diffusion. A chemical solver with general kinetic expressions is coupled to the LBM via mass fluxes at the solid-fluid interface. The mineralogy of the solid is described by scalar fields, each representing a mineral phase. The rate of dissolution or precipitation of a mineral depends on the local chemical disequilibrium and on a kinetic rate constant specific to each mineral.