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Dissolution of a single mineral grain: comparison of microfluidic experiments with pore-scale simulations

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We investigate the dissolution of a single grain of soluble mineral by microfluidic experiments and numerical simulations. The experiments use gypsum cylinders (10 mm radius, 0.5 mm thick) cast from rehydrated CaSO4 hemihydrate. The numerical simulations used a finite-volume discretization of the reactive-transport equations with a mesh that conforms to the evolving shape of the mineral. Using the coefficients for dilute aqueous ions, we overpredict the dissolution rate by about 25%. However, including the Debye-Huckel correction for the ion activity gives a substantial reduction in diffusion across the boundary layer at the dissolving solid surface and brings the simulation time scale into quantitative agreement with experiment.

The asymmetry introduced by the flow causes the initially cylindrical sample to take on a shape resembling one half of a figure eight, with the tip pointing in the downstream direction. The simulations give a near perfect match to the experimental size and shape. We quantify the evolution of the volume of the grain and its surface area, as well as its overall shape as the function of the Peclet number. Next we discuss the differences between the geometric surface area and the reactive surface area of a dissolving grain and explore a potential use of these results to upscale the reactive transport problem and obtain the effective reaction rates in a multi-grain system.