



## **Pore-scale modelling of calcite dissolution by acidic water flow**

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In the context of CO<sub>2</sub> sequestration, an objective is exploring the feasibility of long-term storage (thousands of years) in saline aquifers. This requires a better understanding of the dynamics of chemical processes transforming CO<sub>2</sub> after injection. Reactive flow-through experiments by CO<sub>2</sub>-saturated water have been conducted and followed by X-ray microtomography. Different reaction velocities have been observed on rock surface. Purposes of this study are first to explain these observations and second to allow evolution prediction at macroscopic scale.

In order to understand these observations, a pore-scale finite volume code has been developed. Six constituents (H<sup>+</sup>, OH<sup>-</sup>, HCO<sub>3</sub><sup>-</sup>, Ca<sup>+</sup>, CO<sub>2</sub> and CO<sub>3</sub><sup>2-</sup>) are considered. Assuming electroneutrality of the solution and that in the bulk of the fluid phase we have three chemical reactions at equilibrium (three relations given by mass action law), two transport equations have to be solved to compute the concentrations of the six constituents at each point and each time. In a quasi-static approximation, we consider that transport has no influence on flow (i.e. the velocity of the fluid/solid interface can be neglected). Fluid flow is computed solving Stokes equations with an artificial compressibility algorithm.

Before time t=0, the initial solution is in equilibrium with calcite and at atmospheric partial pressure of CO<sub>2</sub> (pH is around 8). The injected solution is saturated by CO<sub>2</sub> at a larger partial pressure; its pH is around 4. These conditions entail that we can't simply consider that calcite dissolution velocity is proportional to H<sup>+</sup> concentration. It depends also on concentrations of Ca<sup>2+</sup> and CO<sub>3</sub><sup>2-</sup>. This dependency entails strong non-linearities in the resolution of the coupled reactive transport system considered here.

The code has been successfully validated on simple geometries with only one con-

stituent. By working on real media, size grid sensitivity has been highlighted, that shows limitations about size grid in relation to typical pore throat sizes. Moreover, we highlighted problem sensitivity to diffusion for small velocities, when diffusion dominates and controls transport. That has been illustrated through various simple examples.

Finally, we will present how this work can be used in order to implement a change of scale, from pore-scale to macro-scale by a volume averaging method.