Simulation of flow and multispecies reactive transport on pore space images

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Laboratory measurements of mineral dissolution rates differ from those observed in field-scale natural systems [1]. In order to shed light on the source of this discrepancy, we carry out numerical simulations using micro-CT images at the pore scale. While previous works in this area used a particle-tracking method to simulate single-species transport and dissolution of chemically homogeneous rocks [2], this work opts for an Euleurian approach which makes the coupling to a geochemical solver straightforward.

We simulate multispecies reactive flow directly on voxelised pore-space images of consolidated rock obtained from X-ray microtomography. On the initial pore-space geometry, we calculate the steady-state velocity field by solving the Stokes equation using a finite volume method. Then we solve the advection-diffusion equations for the concentration fields. Using a sequential non-iterative approach, we couple the transport solver to a multispecies geochemical solver [3], which was specifically designed for sequential equilibrium problems like the ones that arise from the perturbation of the concentration fields by the advection and diffusion of species. A chemical equilibrium and kinetics problem is solved for each pore voxel, which is considered as a well-mixed batch with an added solid phase if the pore voxel is in contact to a solid voxel. Using this approach, both fluid-fluid and fluid-solid reactions are considered. As dissolution and precipitation take place, the geometry is changed and the velocity and concentration fields are updated accordingly.

The chemical heterogeneity is taken into account by associating each solid voxel to a different mineral and its respective reaction rate. This methodology allow us to simulate fluid-fluid and fluid-solid multispecies reactive transport through chemically heterogeneous rocks, permits pore-by-pore comparison with laboratory experiments on micro-CT images, and can be used to assess the combined effect of physical and chemical heterogeneity on the evolution of dissolution and precipitation.

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