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Dissolution patterns and rates in a heterogeneous limestone studied by using a multicomponent reactive transport model at the pore scale

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Reactive transport modelling at the pore scale explores the spatial-temporal changes in the pore network geometry, the flow field and water composition at sub-centimetre scale. It requires a true representation of fluid-mineral boundaries and their role as zones of fluid-mineral reactions, spatially explicit mass transport and a set of chemical equations to calculate the aqueous speciation and rate of reactions.

We developed a 3D multicomponent reactive transport model by coupling the transport equation solver COMSOL to the geochemical reaction solver iPHREEQC C++ (Parkhurst and Appelo 2013) library using the java-based COMSOL-PHREEQC interface, iCP (Nardi, Idiart et al. 2014). A particular feature of the model is the implementation of the fluid-mineral boundary layer where kinetically controlled mineral dissolution and precipitation can occur.

Flow-through experiments were carried out to study the dissolution of a small bioclastic limestone core from Mt. Gambier, South Australia, through the injection of an acid. The time-dependant pore network geometry of the sample was derived from microCT images and the water composition continuously monitored throughout the experiment. Excellent agreement was found for the whole-core dissolution rate derived from the image-based change in volume fraction, the quantification of dissolved calcium in the outflow and the 3D reactive transport model. Acid buffering through carbonate dissolution strongly controls the dissolution pattern: A high degree of face dissolution as opposed to wormhole formation is observed in sequential microCT images and simulation results. Our study highlights the need to include the aqueous chemical system in reactive transport modelling in order to predict the dynamic changes in dissolution rates and the associated changes in the pore geometry.

References

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