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A 1D plug flow reactor as validation tool for reactive transport simulations

G. Battaïa (1) and D. Garcia (2)

(1) CNRS, BioEMCo, France (guillaume.battaia@grignon.inra.fr), (2) SPIN Generic, Ecole Nationale Supérieure des Mines de Saint-Etienne. France

Predictions in CO₂ geological sequestration involve a broad range of earth sciences linked in complex models. Amongst the processes commonly described, fluid-rock interactions are both a central issue and a source of discomfort for modelers since it has to deal with 1) kinetics data obtained through experimental procedures that dramatically differ from natural systems and 2) reactive surface model that are very diverse and often empirical.

This study presents a new type of plug flow reactor developed to provide an experimental validation of reactive transport simulations. This is a 1D pressurized packed-bed plug-flow reactor containing a granular mixture as a porous medium. This mixture is composed of a reactive solids and unreactive quartz used to set an adequate ratio between fluid and reactive mineral to control the front velocity. A seven sampling valve unit allows concentration profiles of the reacting fluid to be captured at any time.

One the one side, a low reaction rate (diopside, HNO_3 , pH 2) produces linear profile resulting from a constant dissolution rate along the reactor length. But on the other side, when performing the reaction of CO_2 saturated solutions (5 bar) at $40^{\circ}C$ with dolomite it gives rise to dissolution fronts migrating downstream. A proper projection of experimental data reveals a dynamic steady state of front shape is reached. Texture of the mineral recovered at the end of the experiment is quantified by Hg-porosimetry and these results are linked to SEM observations. Altogether, this provides a robust way for the parameterization of a reactive surface area model.