Modeling degradation of cement at different p_{CO2} in flow-through conditions

CHRISTOPH BORKEL[1*], MIREIA GRIVÉ[2] AND
JORDI BRUNO[2]

[1]Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal, Karlsruhe, Germany (*correspondence: christoph.borkel@kit.edu)
[2]Amphos 21 Consulting SL, Barcelona, Spain

We present a reactive transport model (RTM) for degradation of Sulphate Resistant Portland Cement (SRPC) in a modified thin-layer flow-through reactor [1]. In corresponding laboratory experiments CO_2 partial pressure was varied from very low ($CO_2(g)$ <2ppm) to concentrations encountered in granitic groundwater (2mmol/l $HCO_3^-(aq)$). Outflow solutions were closely monitored for pH and released ions from the solid. The modeling aimed to realistically reproduce degradation of the multiphase material, including reprecipitation of secondary phases, as well as removal and transport of ions. Therefore, the initial model composition was mass-balanced with the experimentally employed SRPC. The RTM was realised as a 1-D column using a law of mass action code (Phreeqc [2]). A constant flow rate of 1ml/min was used, causing the necessity to assign kinetic rates to precipitation and dissolution reactions of the solid phases. To determine the necessary column refinement a sensitivity analysis was performed. Corse resolution resulted in relatively well agreement of pH and ion concentrations in outflow concentrations. However, in-detail analysis of individual calculation steps revealed mismatch between calculated saturation states and dissolution/precipitation rections, thus showing a potential pitfall of such a model. Extensive refinement resulted in very long calculation times. The final RTM successfully reproduced degradation of SRPC with four input solutions at different $CO_2(aq)$ content. Modeling results indicated that an earlier drop of pH in outflow solutions with increasing carbonate content was not due to accelerated cement degradation. It was caused by superior buffering capacity of the input solution. With granitic groundwater this occurred to an extent that outflow pH was not representative for the dissolving cement phases anymore.

[1] Bruno, Casas & Puigdomènech (1991), *Geochimica et Cosmochimica Acta* **55**, 647-658
[2] Parkhurst & Appelo (2013), *U.S. Geological Survey Techniques and Methods* **A43**