Integrating high resolution characterization of hydrothermal flow-through experiments into reactive transport simulations of CCUS in sedimentary reservoirs

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Reactive transport modelling is an invaluable tool for analyzing the effect of Carbon Capture, Utilization, and Storage (CCUS) on reservoir chemistry and flow properties. Nonetheless, effective simulation of target reservoirs and their seals often requires the integration and extrapolation of thermodynamic, kinetic, and hydrologic data from many disparate sources. The validity, compatability, and accuracy of these data-model combinations are unfortunately often untestable due to the relative scarcity of appropriate parameterizations in the literature. Here, we present hydrothermal flow-through experiments on K-feldspar-rich sandstone and dolomite core samples and utilize the reactive transport simulator PFLOTRAN[1] to interpret and upscale the experimental results. Using laboratory and synchrotron X-Ray Computed Tomography (XRCT) performed before and after the experiments, fluid chemistry samples obtained throughout the experiments, and a number of other characterization techniques, we monitor the coupled evolution of fluid chemistry and hydraulic properties with reaction progress. We compare porosity and surface area changes measured at the full-core and pore scale as well as core-averaged mineral reaction rates with literature parameterizations and fully coupled numerical experiments. In general, literature parameterizations for mineral reaction rates can be made consistent with our experimental results if adjustments to mineral surface areas are made; however, the evolution of porosity, permeability, and surface area with reaction progress remains considerably more difficult to predict.

[1] Hammond, G. E., Lichtner, P. C., Lu, C., & Mills, R. T. (2012). PFLOTRAN: Reactive flow & transport code for use on laptops to leadership-class supercomputers. *Groundwater Reactive Transport Models*, 142-160.