



Systematic evaluation of experimental parameters and identification of data gaps for geochemical modeling in the context of geological CO₂ storage

Susanne Stadler, Andreas Riße, Katja Heeschen, Heike Rütters, and Christian Ostertag-Henning
Federal Institute for Geosciences and Natural Resources (BGR), Hanover, Germany (susanne.stadler@bgr.de)

Geochemical modeling is an important tool for understanding the interaction of CO₂ with formation fluids and rocks in the context of Carbon Dioxide Capture and Storage (CCS). Plenty of geochemical data exist in the literature, though those are often patchy due to the involved number of components, the broad range of pressure and temperature conditions relevant for geological CO₂ storage and the high salinity of the involved brines. In addition, some parameters have a non-linear dependency, the effects of which have to be considered if extrapolation is attempted to fill gaps not covered by experimental data. We present a compilation of literature data on the experimental solubility of CO₂-H₂O and several mineral-H₂O-CO₂-electrolyte systems within the pT-field of typical potential formation conditions as found in the Northern German Basin. These data will later be used for a simulation of more complex fluid-fluid-mineral interactions that will be conducted within the project COORAL (=CO₂ Purity for Capture and Storage). In our contribution we show a systematic parameter evaluation for data of monomineral interaction with CO₂ in the presence of defined electrolyte solutions. We show results of a set of experiments of up to 768 h duration at 200 bar and 120°C (with 150 g/L NaCl) where we added and/or varied specific controlling factors. The experimental data are compared with modeling results applying the geochemical simulator PHREEQC. In addition to thermodynamic calculations, we test variations in experimentally derived rate parameters for their sensitivity in kinetic calculations.