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Uncertainties in geochemical modeling using different software programs and thermodynamic datasets

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For simulating water-mineral interactions following a CO2 sequestration into deep saline aquifers within numerical reactive transport models, parameters like the model program, the thermodynamic databases, or secondary minerals have to be selected. These parameters used include uncertainties which are known in general, but are not quantified in detail and their impact on reaction calculations in the field of CCS is rarely discussed. One major aim of the CO2-MoPa joint research project is to identify the key parameters which influence water-mineral interactions in numerical CO2 storage models significantly. The significance of the geological and the calculative variances needs to be evaluated with respect to typical timescales relevant for CCS measures.
Because simple comparisons of for example equilibrium constants in databases were not meaningful in terms of determining the key parameters, we have performed sensitivity analyses to identify and quantify these key parameters. The results indicate that the influence of the geochemical modeling program used (PHREEQC, EQ3/6, Geochemist's Workbench, FactSage/ChemApp) is comparably low. In general, variances of calcite dissolution in model results using the different thermodynamic datasets rise with the salinity, the CO2 fugacity (1 to 100 bars), but decrease with temperature (25-75°C). For example in a set of scenario analyses with the boundary conditions of an ionic strength of 0.5 M, T = 25°C, and fCO2 = 100 bars, the calculated amount of dissolved calcite ranged between 1 and 126 mmol/L using the 26 evaluated thermodynamic databases. The use of mono-valent kations (Na+) together with chloride as the anion as the background electrolyte causes the variation of the calculated reactions to be less profound than the use of di-valent kations (Mg++) together with chloride.
During scenario analyses modeling the virtual CO2 injection into a test site, the use of thermodynamic constants generated with SUPCRT92 in order to adjust for temperature and pressure conditions caused the model results to be divergent from results obtained using original PHREEQC databases. Because the influence of a pressure correction of equilibrium constants was comparably low, it is uncertain if the pressure correction, and so the use of the SUPCRT92 database, has to be valued higher than regarding calculation uncertainties caused by the use of either of the original PHREEQC thermodynamic databases. The choice of possible secondary minerals like kaolinite, illite, or dawsonite, influences the model results even stronger. The production of dawsonite during the reactions following the injection of CO2 has not been proven so far. Including the mineral dawsonite, increased the maximum amount of fixed CO2 in the scenario analyses by up to factor two. This uncertainty has to be regarded additionally in the setup of reactive transport models.