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## Uncertainties in Hydrogeochemical Modelling of Water-mineral Interaction in the Field of CO2-storage

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## SUMMARY

Modelling of water-mineral interactions in deep saline aquifers following an injection of CO2 shows significant dependence on the applied software and thermodynamic dataset. Five scenarios were used to calculate the precipitation or dissolution of a mineral and each scenario was modelled with the programmes and their provided thermodynamic datasets.

Four different hydrogeochemical modelling programmes, PHREEQC, EQ3/6, The Geochemist's Workbench and FactSage/ChemApp, were used. While the first three programmes compute the equilibrium state based on the equilibrium constant approach, FactSage minimizes the Gibbs energy to reach the equilibrium state. Comparisons of the programmes using the same thermodynamic dataset show that the modelling results are similar.

In four out of five modelled scenarios hypothetical groundwater compositions consisting of major cations and anions in ionic strengths of 0.04 and 0.6 mol/l, respectively, were used. Selected temperatures were 25 and 60°C, respectively, and the CO2 fugacity was fixed at 10 bars. For the fifth scenario a brine of Lower Cretaceous sediments at reservoir conditions was used. In this case CO2 fugacity was fixed according to a depth of approximately 1000 m. In all of the scenarios the dissolved or precipitated amount of various minerals was calculated, which typically occur in the sediments of northern Germany and which are in addition important for the mineral trapping of CO2.

The results of the first four scenario calculations show exemplarily for calcite that at the low ionic strength of 0.04 mol/l and both given temperatures the amount of dissolved calcite varies from $8.4 \times 10^{-3}$ to $1.7 \times 10^{-2}$ mol at 60°C between the dataset "llnl.dat" of PhreeqC and "FT_Helg" of Factsage. At the higher ionic strength of 0.6 mol/l a dissolution of calcite with a variation from $5.5 \times 10^{-2}$ to $6.3 \times 10^{-2}$ was calculated by using three of the 22 thermodynamic datasets. By using the other 19 datasets calcite precipitates by $3.5 \times 10^{-3}$ to $7.8 \times 10^{-3}$ mol instead of being dissolved. In the fifth scenario the variation of the amount of dissolved calcite ranges from $3.8 \times 10^{-3}$ to $2.2 \times 10^{-2}$ mol.

This discrepancy is caused by different aqueous complexes and their equilibrium constants, which are differing in the used datasets.

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