How to implement temperature-dependent Pitzer interaction coefficients into TOUGHREACT?

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Final disposal of radioactive waste is foreseen in a deep geological formation in Germany. Salt, clay and granite formations are possible host rocks.

Solutions with high ionic strength occur naturally in salt formations. Also formation waters of clay rocks and granites can have a high ionic strength in the northern part of Germany. The Pitzer approach using ion interaction parameters is used for the calculation of the aqueous composition and the saturation state relative to a set of minerals for high saline solutions. The THEREDA project [1] provides a consistent thermodynamic database with ion interaction parameters (Pitzer) for different geochemical codes (e.g. PHREEQC, ChemApp and EQ 3/6). Already nine releases for geochemical systems are published.

We plan to use data sets from THEREDA with TOUGHREACT [2] and to compare existing modeling results from our in-house code MARNIE [3] coupled with PHREEQC and ChemApp using identical data sets for verification.

The implementation of the ion interaction parameters in TOUHGREACT v1.2 uses a polynomial fit with four coefficients to describe the temperature dependence $[X(T) = a_1 + a_2 \cdot (1/T - 1/T_0) + a_3 \cdot \ln(T/T_0) + a_4 \cdot (T-T_0)]$, whereas THEREDA uses a fit having six coefficients $[X(T) = a/T + b + c \cdot \ln(T) + d \cdot T + e \cdot T^2 + f/T^2]$. This applies similarly for log K where TOUGHREACT uses five and THEREDA six coefficients for fitting. In order to avoid potential inaccuracies of a conversion, it is foreseen to implement the polynomial fit with six coefficients (a-f) in TOUGHREACT.

Furthermore it is also planned to add the Pitzer approach in TOUGHREACT v3 [4] to carry on the application of reactive transport models on high ionic strength solutions in salt and clay rocks for long-term safety analysis.

The implementation of the polynomial fit function as well as first modeling results will be discussed.

[1] www.thereda.de/en/;
[2] TOUGHREACT V1.2 Pitzer, LBNL-62718, 2006.
[3] GRS-334, ISBN 9783944161143, 2014.
[4] TOUGHREACT V3.0-OMP. LBNL-DRAFT, 2014.