Geophysical Research Abstracts
Vol. 13, EGU2011-13903, 2011
EGU General Assembly 2011

A geochemical model for highly saline solutions

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In Germany anhydrous MgSO4 (SVV) is considered as potential sealing material for the isolation of High-Level-Waste (HLW) in salt rock. When brine approaches the sealing material (SVV), different MgSO4-hydrates along with other mineral phases (e.g. bloedite) form, removing free water from the solution. This leads to a situation with little or no free water. The uptake of water leads to an overall increase of solid phase volume. If deformation is constrained, the pore volume decreases and permeability is reduced. In order to simulate such processes, especially for conditions without free water, a coupling between the object-oriented programming (OOP) FEM simulator OpenGS and the commercially available thermodynamic simulator ChemApp was implemented. ChemApp uses the Gibbs Energy Minimization (GEM) approach for geochemical reaction simulation. Based on this method, the thermodynamic equilibrium of geochemical reactions can be calculated by giving the amount of each system component and the molar Gibbs energy of formation for all the possible phases and phase constituents. Activity coefficients in high-saline solutions were calculated using the Pitzer formalism. This model has the potential to handle 1D, 2D and 3D saturated and non-saturated thermo-hydro-chemical (THC) coupled processes even with highly saline solutions under complex conditions. The model was verified by numerical comparisons with other simulators (e.g. EQ3/6) and applied for the modeling of SVV experimental data.