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Development of a new activity model for complex mixed-salt solutions from ambient to geothermal conditions

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Geochemical modeling of fluid-rock interaction in geothermal environments is a demanding task because of the prevalent high temperatures, pressures and salinities. Solution speciation, mineral compositions and assemblages as well as gas compositions are typically computed from multicomponent-multiphase thermodynamic models for standard state properties and activities or fugacities. In concentrated aqueous solutions, the Pitzer model (Pitzer, 1973) is the standard approach for computing solute species and solvent activities. An alternative model is the extended universal quasichemical (EUNIQUAC) model (Thomsen & Rasmussen, 1996).

The Pitzer model is based on a virial expansion of the osmotic pressure. For complex multi-electrolyte solutions comprising several dozens of solute species, the number of empiric parameters for the Pitzer model can easily excceed several hundreds. The EUNIQUAC model needs less than a quarter of the empiric parameters required for the Pitzer model. EUNIQUAC is based on more recent theoretical approaches to the statistical mechanical treatment of solutions. A disadvantage of the EUNIQUAC model is that it gives a less accurate representation of the experimental data. A disadvantage of both models is that they are typically only parameterized along the vapor-pressure saturation curve, which considerably restricts their range of application at geothermal conditions.

We developed a modification of the EUNIQUAC model (termed ELVIS) which preserves the non-electrostatic framework of EUNIQUAC, but accounts better for electrostatic interactions. ELVIS needs significantly fewer parameters than the Pitzer model, but yields comparably accurate representation of experimental data. Unlike the EUNIQUAC and Pitzer models, the ELVIS parameters are formulated both in terms of temperature and pressure dependence. First results of calibrating the ELVIS model to experimental data of the H_2O-NaCl and H_2O-CaCl2 systems over wide ranges in temperature, pressure and composition are presented.

References:
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