A new aqueous activity model for geothermal brines in the system Na-K-Ca-Mg-H-Cl-SO4-H2O from 25 to 300 degrees C

A revised formulation (named REUNIQUAC) of the Extended Universal QUasiChemical (EUNIQUAC) activity model has been developed, which fits excess thermodynamic properties of binary and selected aqueous ternary electrolyte solutions in the system Na-K-Ca-Mg-H-Cl-SO4-H2O over temperatures from 298 to 573 K and concentrations to 5 molal (or up to saturation if solubility is below 5 molal) for saturated water vapor conditions. Compared to the original EUNIQUAC model, REUNIQUAC employs an extended version of the Debye-Huckel model using effective ionic radii of solute species, a concentration dependence of a UNIQUAC parameter, an additional empirical term for strongly complexing salts, as well as a simple quadratic temperature dependence of the fitting parameters. REUNIQUAC considers only pairwise interactions between solute species, as opposed to the Pitzer activity model, which additionally needs to account for ternary interactions. Since REUNIQUAC uses also species-specific parameters, extension of the existing parameter set to solutions that are composed of different combinations of the fitted species, is straightforward, and involves only the parameterization of the pairwise interaction terms. All systems could be fitted with accuracy comparable to the Pitzer model or better, although with much fewer parameters.

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