

Use of UNIQUAC's Model to Calculate mineral solubilities in Aqueous Electrolyte solutions of Ternary Systems

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Abstract

The activity coefficients of ions in the several ternary systems have been calculated by the UNIQUAC model. Using these values of activity coefficients in the equilibrium equation, the solubilities of solids in the aqueous electrolyte solutions have been calculated. These calculations are performed for $\text{Na}_2\text{SO}_4\text{-NaCl-H}_2\text{O}$, $\text{Na}_2\text{SO}_4\cdot 10\text{H}_2\text{O -NaCl-H}_2\text{O}$, $\text{K}_2\text{SO}_4\text{-KCl-H}_2\text{O}$ and $\text{K}_2\text{SO}_4\text{-Na}_2\text{SO}_4\text{-H}_2\text{O}$ systems. The comparison of the calculated results with the experimental data shows that the UNIQUAC model is able to give a good representation of the solid-liquid phase equilibria in these mineral solutions in the whole temperature range from 273.15 to 373.15K.

Key words: SLE calculation; UNIQUAC model; electrolyte solutions.

Introduction

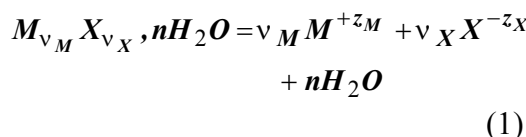
The correlation and prediction of phase equilibrium data are of major importance in the design of equipment for separation processes in the chemical industries. For non-electrolyte mixtures at ordinary temperature and pressure, reliable models are available today. For electrolyte mixtures, several research works have done to understand the thermodynamic properties of aqueous mixtures in the last decades, and progress has been made in the development of theories for electrolyte solutions. Examples of previous works are the extensive work of Pitzer and co-workers [1-4] and Sander [5] and Lu and Maurer [6-7]. In the work of Sander, the extended UNIQUAC model was used for prediction of SLE for electrolyte solutions. For more information, review paper of Loehe and Donohue is a good reference [8].

The objective of this study is to investigate the ability of the extended UNIQUAC model for calculations of solid-liquid equilibrium for ternary systems of $\text{K}_2\text{SO}_4\text{-KCl-H}_2\text{O}$, $\text{Na}_2\text{SO}_4\text{-NaCl-H}_2\text{O}$,

$\text{Na}_2\text{SO}_4\cdot 10\text{H}_2\text{O -NaCl-H}_2\text{O}$ and $\text{K}_2\text{SO}_4\text{-Na}_2\text{SO}_4\text{-H}_2\text{O}$. The calculated results are compared with the experimental data reported in the literature [9].

Theory

For a solid with a composition $\text{M}_{v_M}\text{X}_{v_X}\cdot n\text{H}_2\text{O}$, which consists of v_M positive ions, M, of charge z_M , v_X negative ions, X, of charge z_X and n crystal water, the equilibrium constant, K, for the dissolution reaction



is given by:

$$\ln K = \mu_s^o / RT - (v_M \mu_M^o + v_X \mu_X^o + n \mu_w^o) / RT \quad (2)$$

where the μ_i^o 's are the chemical potentials of the solid or of the aqueous species at their defined standard states.

In term of activity coefficients, the equilibrium constant of above reaction is given by: