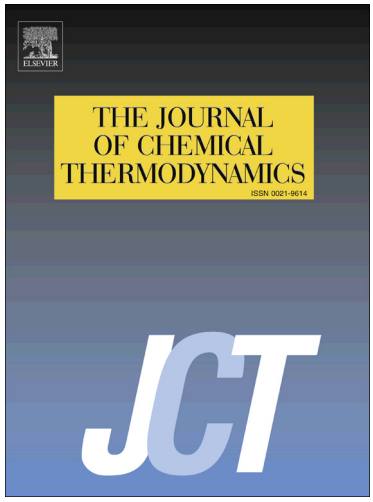

A thermodynamic model for molten salt-water solutions – Application to a thermodynamic optimization of the $Ca(NO_3)_2$-KNO_3-H_2O system

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A thermodynamic model for molten salt-water solutions – Application to a thermodynamic optimization of the $Ca(NO_3)_2$-KNO_3-H_2O system

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ABSTRACT

A new thermodynamic model has been developed for molten salt-water solutions. The model applies particularly to salt-rich solutions but may be applied over the entire composition range from anhydrous salts to pure H_2O. The model is an extension of the two-sublattice Modified Quasichemical Model for molten anhydrous salt solutions with first-nearest-neighbour short-range ordering. The model assumes the existence of hydrated cations such as $K(H_2O)_j^+$ and $Ca(NO_3)_k^{2+}$ as well as "free" neutral H_2O molecules. The model has been used in a complete critical evaluation and thermodynamic optimization of the three binary systems KNO_3-$Ca(NO_3)_2$, KNO_3-H_2O and $Ca(NO_3)_2$-H_2O and of the ternary system $Ca(NO_3)_2$-KNO_3-H_2O.

Keywords: Molten salt-water solutions, thermodynamic model, Modified Quasichemical Model, $Ca(NO_3)_2$-KNO_3-H_2O system

1. Introduction

Salt-water systems are important in the fertilizer industry. Phase diagrams and the thermodynamic properties of systems relatively rich in salt are of much interest for the production of nitrate-based fertilizers. To this end, we have undertaken a program to develop evaluated optimized thermodynamic databases for salt-H_2O systems similar to those developed by our research group over many years for systems of anhydrous salts, oxides, metals, etc [FactSage]. From these databases, thermodynamic properties and the conditions for phase equilibria can be calculated.

In such databases, the thermodynamic properties are stored in the form of parameters of models for each phase. However, for molten salt-H_2O solutions, no satisfactory model has been available which is applicable at compositions up to and including the pure anhydrous salts.. Several successful and well-developed models exist for solutions of salts in water [91Pit, 85Bow, 2002Wan]; however these models apply only to solutions relatively rich in H_2O (up to approximately 30 molal.). Thermodynamic models also exist for anhydrous molten salt solutions. These are generally two-sublattice models with cations assumed to occupy one sublattice and anions the other [64Bla, 74Sab, 2001Cha-a, 2001Pel-a, 85Hil].

In the present article a new thermodynamic model is developed for molten salt-water