

138d Statistical Associating Fluid Theory Coupled with Restricted Primitive Model to Represent Aqueous Strong Electrolytes: Multiple-Salt Solutions

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Aqueous electrolyte solutions, especially aqueous multiple-salt solutions, are encountered in wastewater treatment, extraction, seawater desalinization, and distillation. In enhanced oil recovery by water flooding, the composition of the connate and invading brines could have a major influence on wettability and consequently improve the oil recovery at reservoir temperature. In enhanced oil recovery by CO₂-flooding, the presence of salts in water reduces the solubility of CO₂ in water. As indicated in a simulation study, the oil recovery increases with the salinity of the brines. Despite of their important role, the modeling of aqueous electrolyte solutions, especially multi-salt solutions, is still a challenging task.

We proposed Statistical Associating Fluid Theory coupled with MSA, specifically with the Restricted Primitive Model (RPM), referred to as SAFT1-RPM, which was found to represent the mean activity coefficients, osmotic coefficients, vapor pressures, and densities of aqueous one-salt solutions of alkali halide [1]. In this work, we extend this model to multiple-salt solutions using a mixing rule for the hydrated diameter. A binary adjustable parameter in this mixing rule, for a pair of salts, is obtained from experimental osmotic coefficients of the corresponding two-salt system. The two-salt systems considered contain water and possible pairs of NaCl, KCl, NaBr, and KBr. LiCl+NaCl and LiCl+KCl pairs are also correlated. The adjustable parameters are used to predict the density of the two-salt systems with or without common ions, the solubility of two two-salt systems, and the osmotic coefficient of a quaternary NaCl-KCl-LiCl-H₂O solution.

[1] Tan, S.P.; Adidharma, H.; Radosz, M. Statistical Associating Fluid Theory Coupled with Restricted Primitive Model To Represent Aqueous Strong Electrolytes. *Ind. Eng. Chem. Res.*, 2005, in print.