

Statistical Associating Fluid Theory Coupled with Restricted Primitive Model to Represent Aqueous Multiple-Salt Solutions

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Aqueous electrolyte solutions, especially aqueous multiple-salt solutions, are encountered in wastewater treatment, extraction, seawater desalinization, distillation, and oil recovery. In oil recovery by water flooding, the composition of the connate and invading brines can affect wettability and hence 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, and hence the oil recovery increases with increasing brine salinity.

Statistical Associating Fluid Theory (SAFT) coupled with Restricted Primitive Model (RPM) is used to represent the properties of such multiple-salt solutions. The water is modeled as a spherical molecule with four associating sites and the ion is modeled as a non-associating spherical molecule with a charge. One set of parameters is derived from the available experimental mean ionic activity coefficients of the salt and from the density of single-salt solutions at 25°C composed by Li, Na, K, Ca²⁺, Mg²⁺, Cl⁻, Br⁻, I⁻, NO₃⁻, SO₄²⁻, HCO₃⁻, and CO₃²⁻. Without any additional adjustments, these parameters are used to predict the osmotic coefficients and vapor pressures of single-salt solutions, and to predict the osmotic coefficients, vapor pressures, densities, and activity coefficients of multiple-salt solutions. We shall explore the high temperature and high pressure properties of such solutions.