148p Saft1-Rpm Equation of State: Application to Phase Equilibria and Thermodynamic Properties of Carbon Dioxide + Aqueous Electrolyte Solutions

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The knowledge of the solubility of carbon dioxide in aqueous electrolyte solutions is of considerable interest to petroleum and gas industries. For example, in the enhanced oil recovery using carbon dioxide flooding, the solubility of carbon dioxide in the connate water (brine) reduces the amount of CO2 available for miscible oil displacement, which in turn affects the oil recovery. Another example, the existence of electrolytes is known to affect the solubility and selectivity of CO2 and other natural gas components in the equilibrium phases, especially in the low-temperature region close to the hydrate formation, the knowledge of which has a potential application in gas separation technology. In the CO2 sequestration in saline formations and oceans, the knowledge of the solubility of carbon dioxide in brine is also an important factor.

In this work, we use the Statistical Associating Fluid Theory coupled with Restricted Primitive Model (SAFT1-RPM) [1] for representing CO2-H2O-NaCl system. For pure components, CO2 molecule is modeled as a molecule with three association sites, i.e., two sites of type O and one site of type C and H2O molecule is modeled as a molecule with four association sites, i.e. two sites of type O and two sites of type H. Parameters of pure CO2 are fitted to vapor pressure and liquid density data. The parameters for H2O and NaCl have been obtained in our previous work [1].

For CO2-H2O system, we assume that there is only one type of cross association, i.e., between site of type O in CO2 and site of type H in H2O. The cross association between site of type C in CO2 and site of type O in H2O is considered weak and negligible. The temperature dependences of the binary interaction parameters for this system are fitted to the experimental equilibrium compositions of CO2-rich and H2O-rich phases from 12 to 200ºC and pressure up to 600 bar. The SAFT1 model is found to represent the equilibrium data, including the minimum H2O concentration in the CO2-rich phase in the P-y diagram. For CO2-H2O-NaCl system, we use one additional constant binary interaction parameter for both CO2-Na+ and CO2-Cl- pairs, which is needed to correct the short-range interactions. The SAFT1-RPM model is found to represent the equilibrium data up to molality of 6 mol/kg. The predictability of the model for the density calculations of these systems is also discussed.

[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.