Calculation of Hydrate-Containing Phase Equilibria Using Electrolyte Equation of State Based on Hydrogen-Bonding Nonrandom Lattice Fluid Model

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In carbon dioxide sequestration process, captured carbon dioxide may contain small amount of water and sulfur dioxide as impurities, forming gas hydrate under the hydrate stability condition. For such mixtures of carbon dioxide, sulfur dioxide and water, modeling study on the hydrate phase equilibria has not been reported to present. Sulfur dioxide in aqueous solution is partially dissociated as weak electrolyte. In this study, the electrolyte equation of state based on hydrogen-bonding nonrandom lattice fluid theory (Electrolyte NLFHB EOS) was employed and extended to the weak electrolyte solution. In the model, the contribution of long-range interaction from mean spherical approximation (MSA) was added to original equation of state for nonelectrolyte components. Various phase behavior with and without gas hydrate was successfully analyzed using the model.