Hydrate Based Desalination: Thermodynamic and Kinetic Perspective

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Water scarcity is becoming a severe problem worldwide because of the inadequate freshwater resources and swift population growth. Seawater desalination is one of the vital approaches to meet the demand for freshwater. However, energy and associated costs with the conventional seawater desalination techniques pushed towards the use of non-conventional water desalination processes. Water desalination using gas hydrates formation is one of the emerging non-conventional processes. However, limited control in the separation of hydrate crystals, salt deposition on hydrate particles, and hydrate morphology prevented the commercialization of the hydrate-based desalination process besides promising results on salt removal efficiency. The kinetics of hydrate formation was investigated with the possibility of zero induction regime and controlled hydrate morphology.

Moreover, In the design of any hydrate-based desalination, accurate prediction of the phase behavior of the hydrate former (*HF*) + salts + water systems is critical to evaluate the pertinent driving force/subcooling, type of hydrate structure and fractional cage occupancy, phase amounts (at equilibrium), optimal cage/HF composition, and suitable hydrate dissociation conditions. The use of the Broomley activity model coupled with modified van der Waals-Platteeuw (*vdWP*) theory (*CSMGem*) leads towards the higher absolute average deviation (*AADP*) for high salt concentrations, 1:2 electrolytes, and mixed salt systems. In this work, various other electrolyte models: Debye Huckel, truncated Debye Huckel, and Pitzer theory were also coupled with the *GEM* algorithm for hydrate phase equilibria calculations. The hydrate phase equilibria predictions were conducted with former physical models for various salts over various concentrations and charge density. Furthermore, a more rigorous statistical thermodynamics approach (Mean Field Spherical Approximation) was also developed to accurately predict the activity of the aqueous phase and phase behavior of salt-containing systems for high salt concentrations and mixed salt systems.