Development of a Comprehensive Molecular Thermodynamic Model for High Salinity Produced Water in Oil and Gas Productions

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Abstract

Managing produced water in the rapidly developing shale gas industry is a major challenge for protecting the environment [Shaffer et al., *Environ. Sci. Technol.* 2013, 47, 9569-9583]. Desalination for reuse of produced water depends on novel material and process innovations. We present progress in the development of a comprehensive thermodynamic model aimed to support heat and mass balance calculations and process simulation of desalination processes with produced water. Based on the electrolyte Non-Random Two Liquid theory (eNRTL) for electrolyte solutions [Song and Chen, *Ind. Eng. Chem. Res*. 2009, 48, 7788-7797] , the model intends to cover major ions of concern for produced water management: Na^+, K^+, Mg^{2+}, Ca^{2+}, Ba^{2+}, Sr^{2+}, Cl^-, HCO_3^- and SO_4^{2-} ions. In the thermodynamic framework of eNRTL, the concentration dependency of the solution nonideality is accounted for with two binary interaction parameters for each of the water−electrolyte interaction pairs and the electrolyte–electrolyte interaction pairs. The temperature dependency of the binary interaction parameters is accounted for with a Gibbs-Helmholtz type expression with three temperature coefficients representing excess Gibbs energy, excess enthalpy, and excess heat capacity contributions. With the binary parameters regressed from thermodynamic data of aqueous single electrolyte binary systems and aqueous two electrolyte ternary systems, the model has been shown to provide accurate calculations and reliable predictions for various thermodynamic properties of quaternary and quinary systems examined thus far for the aqueous Na^+−K^+−Mg^{2+}−Ca^{2+}−Cl^-−SO_4^{2-} hexary system with temperatures from 273.15 K to 473.15 K and concentrations up to salt saturation. The model is being extended to cover Ba^{2+}, Sr^{2+} and HCO_3^- ions and it should become an indispensable scientific tool in the development of novel desalination processes for high salinity produced water in oil and gas productions.