

Temperature Dependency of Interaction Parameters of Electrolyte NRTL Model

Nazir Hossain^S, Sanjoy Bhattacharia and Chauchyun Chen^C
Chemical Engineering, Texas Tech University, Lubbock, Texas, U.S.A.
chauchyun.chen@ttu.edu

Accurate thermodynamic modeling of aqueous electrolyte solutions is essential for many industrial applications such as hydraulic fracturing, desalination, nuclear waste management, etc. Requiring only two binary interaction parameters, the electrolyte non-random two liquid (eNRTL) model is capable of representing the liquid phase nonideality over the entire concentration range from pure water to pure fused salt. Another important characteristic of the eNRTL model is the weak temperature dependency of the binary interaction parameters. In this study we investigate the relationship between temperature coefficients of the eNRTL binary interaction parameters and excess molar enthalpy of electrolyte solutions. We show excess molar enthalpy of electrolyte solutions form a simple family of curves as function of electrolyte concentration. We further show the temperature dependency of the eNRTL binary interaction parameters can be expressed in a Gibbs-Helmholtz type expression with three temperature coefficients representing Gibbs energy, enthalpy, and heat capacity contributions. The enthalpy term of the temperature dependency expression has been correlated to excess molar enthalpy of electrolyte solutions for more than 100 electrolytes. The resulting eNRTL model and model parameters provide a comprehensive thermodynamic framework to represent all thermodynamic properties of aqueous electrolyte solutions including vapor pressure depression, mean ionic activity coefficients, osmotic coefficients, excess enthalpy, and heat capacity.