

G^{ex} -Model Using Local Area Fraction for Binary Electrolyte Systems

A. Haghtalab¹ and M. Joda^{C,S,2}

¹*Department of Chemical Engineering Faculty of Engineering, University of Qatar, Doha, Qatar*

²*Tehran Oil Refining Company, Tehran, Iran
ahaghtalab@qu.edu.qa*

The correlation and prediction of the phase equilibrium of electrolyte systems are essential in the design and operation of many industrial processes such as down stream processing in biotechnology, desalination, hydrometallurgy etc.

Haghtalab and Vera developed the NRTL-NRF local composition model for binary aqueous electrolyte systems from dilute solution up to saturation point of the salts. In this work, based on NRTL-NRF assumptions, two new excess Gibbs free energy (g^{ex}) functions were derived using local area fraction with assumption of equality or inequality of surface areas of anion and cation, respectively. The modified NRTL-NRF models consist of two contributions due to long-range forces, represented by the Debye-Huckel theory, and to short-range forces, represented by local area fractions of species through nonrandom factors. Each model contains only two adjustable parameters per electrolyte. In addition, the model with unequal surface area of ionic species presents better results in comparison with the second new model with equal surface area of ions. The results of mean activity coefficients for aqueous solution of uni-univalent electrolyte showed that the present model is more accurate than original NRTL-NRF model.