Excess Enthalpy Predictions Using Association NRTL Model for Alcohol-Water-Hexane Mixtures

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Thermodynamic solution models are indispensable for delineating fluid phase equilibria and the thermodynamic properties of liquid systems. The Non-random Two Liquid (NRTL) theory is a local composition model established by Renon and Prausnitz (1968) that employs binary interaction parameters to capture the nonideality due to interactions among components in a mixture. This model is distinguished by its empirical accuracy in correlating binary mixtures' behaviors from vapor-liquid equilibrium (VLE) data. Nonetheless, the extrapolation of NRTL to ternary mixtures, its regression with liquid-liquid equilibrium (LLE) data, or its utilization in predicting excess enthalpy may result in marked deviations from experimental observations. Hao and Chen (2019, 2021) posited that these discrepancies in associating systems arise from an inadequate depiction of hydrogen bonding in the classical NRTL formulation. Their research synthesized NRTL with Wertheim's perturbation theory to account for associative interactions, presenting an efficacious algorithm for applying Association theory. Furthermore, Hao and Chen's model yielded predictions that markedly improved the correlation of LLE data and the characterization of ternary mixtures, as validated by empirical evidence, relative to antecedent applications of the NRTL model. However, their analysis was restricted to mixtures incorporating a singular strong associative component. The current study extends Hao and Chen's approach by extending the association NRTL model to binary and ternary systems with multiple potent associative entities, exemplified by water-alcohol and water-hexane-alcohol mixtures, and evaluates their behaviors against VLE, LLE, and excess enthalpy empirical data sets.

References

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