544g Generalized Uniquac-Qspr Model for Vapor-Liquid Equilibria Prediction of Binary Mixtures

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Multiphase equilibria are at the heart of numerous industrial processes. Several accurate experimental techniques have been developed for measurement of vapor-liquid and equilibrium (VLE) data. However, experimental techniques are often time consuming and expensive. As such, reliable generalized equilibrium models that reduce the experimental burden in phase equilibria modeling have been sought for a priori prediction of VLE phase behavior of targeted systems.

The universal quasi-chemical (UNIQUAC) activity coefficient model is widely used in the chemical industry to handle non-ideal vapor-liquid and liquid-liquid equilibrium systems. Generalized-parameter predictions based on this model through the UNIFAC group-contribution methodology have been useful for many systems that lack experimental data. However, group-contribution models often utilize the first-order approximation for additive structural contributions, which fail to capture the structural subtleties of some of the chemical species considered.

In this work, we develop quantitative structure-property relationships (QSPR) models for a priori predictions of the UNIQUAC model parameters. An extensive database encompassing a wide variety of chemical structures has been used in this model development effort. This work constitutes an extension of our previous QSPR modeling efforts dealing with QSPR modeling of the non-random two-liquid (NRTL) model parameters and pure-fluid saturation properties.