Simple Generalized Expressions Based on a Cubic Equation of State to Represent the Liquid-Liquid Equilibria of High-Polar Substances/Alkane Binary Mixtures

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A simple model based on a two-parameter cubic equation of state and the Huron-Vidal-NRTL mixing rules is used to describe the liquid-liquid equilibria (LLE) of binary mixtures formed by a high polar substance and alkanes. The polar substances included in this study are acetonitrile, propanenitrile, n,n-dimethylformamide, e-caprolactam, benzaldehyde , acetophenone, and n,n-dimethylacetamide. For each polar compound and the homologous series of n-alkanes from C4 to C16, the NRTL binary interaction parameters (A_{12}, A_{21}, α_{12}) are generalized in terms of the temperature, the critical temperature, and the critical pressure. The parameters of the generalized expressions are determined minimizing the total absolute relative deviation in liquid phase molar fraction. To validate the expressions, some predictive calculations that include vapor-liquid-equilibria (VLE), vapor-liquid-liquid equilibria (VLLE), and liquid densities are performed. Results are compared with those reported in the literature for a more complex model like SAFT. Considering the simplicity of the proposed model, the results are adequate for practical purposes. For liquid-liquid equilibria, absolute deviations in the liquid phase molar fraction are in general below 0.041. For VLE and VLLE, the average absolute deviations in bubble pressure are between 3.0 % and 16.2 %. Finally, for liquid densities, average absolute deviations are around 2.0 % at least at nearly room temperature.