Effect of Surface Area Parameters on the Vapor-Liquid Equilibrium Calculations using Lattice Equation of State with Hydrogen Bonding

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Comprehensive vapor-liquid equilibrium calculations were performed using the lattice fluid equation of state with hydrogen bonding (NLF-HB EOS) proposed by Lee and coworkers (You et al., 1996, Lee et al., 2002). Vapor-liquid equilibrium calculations composed of 21 typical pure components were compared with large electronic experimental database (Dortmund Data Bank). Special attention has been paid to the correction of surface area parameters. Bulkiness factors can be used to modify theoretical surface area parameters for molecules with nonlinear shapes. Empirical bulkiness factors were obtained from VLE data sets with n-hexane chosen as a reference component. Using empirical bulkiness factors, the overall prediction performances without binary interaction parameters have been significantly improved. It is shown that the NLF-HB EOS have comparable prediction capability with UNIFAC method only with pure component parameters and component-type-dependent hydrogen bonding energy parameters for most systems considered in this study.