The Effect of Surface Area Parameters on Vapor-Liquid Equilibrium Calculations using a Lattice Fluid 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 a large electronic experimental database (the Dortmund Data Bank). Special attention was 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, overall prediction performances without binary interaction parameters have significantly improved. It is shown that the NLF-HB EoS has comparable prediction capability with the UNIFAC method, for only pure component parameters and component-type-dependent hydrogen bonding energy parameters, for most systems considered in this study.