A Quasi-Chemical Nonrandom Lattice Fluid Hydrogen Bonding Theory for Phase Equilibria of Associating Systems

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Veytsman statistics for the hydrogen bonding contribution is combined with the quasi-chemical nonrandom lattice fluid (QLF) model developed recently by the present authors. The physical contribution is characterized by three temperature-independent molecular parameters representing the close-packed volumes of a n-mer, segment numbers, and interaction energy for a pure fluid, and a binary interaction parameter for a binary mixture. The chemical part is represented by the internal energy and the entropy of hydrogen bonding. The resulting QLF-HB equation of state was applied to describe thermodynamic properties of pure fluids and phase equilibria of mixtures. The results for alkane-alkanol and alkanol-alkanol mixtures showed significant improvements over those of the QLF EoS (equation of state) and the NLF-HB (nonrandom lattice fluid hydrogen bonding) EoS.