Liquid-Liquid Equilibrium of Hydrocarbon-Alcohol Mixtures using Nonrandom Lattice Fluid Equation of State with Hydrogen Bonding

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Nonrandom lattice equation of state with hydrogen bonding (NLF-HB EOS) was examined for the prediction of liquid-liquid equilibria (LLE) for binary alcohol and hydrocarbon mixture at low to high pressure. For hydrocarbon + alkane mixtures, inclusion of hydrogen bonding term in lattice equation of state clearly improves prediction for vapor-liquid equilibrium (VLE) as shown in previous works, but the prediction of LLE is still in question.In this paper, LLE data for alcohol (methanol and ethanol) + hydrocarbon (hexane to hexadecane) were correlated by NLF-HB EOS and results were compared with cubic equation of state (Peng-Robinson with Wong-Sandler mixing rule, PR-WS EOS). Both equations of state showed similar degree of accuracies but with different number of adjustable parameters. PR-WS EOS requires six temperature dependent coefficients for accurate calculation whereas NLF-HB EOS requires only two to three temperature coefficients. Also, effects of varying hydrogen bonding energies and surface area parameters for NLF-HB EOS were discussed.