Vapor-Liquid Equilibria of Real Mixtures with Polar Two-Center Lennard-Jones Models

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Molecular models show a remarkable predictive power regarding thermo-physical properties. On the other hand knowledge on vapor-liquid equilibria of mixtures of real substances is of crucial importance in many fields of process engineering. Hence, it is attractive to systematically study the performance of molecular models in predicting vapor-liquid equilibria and compare it to equations of state.

In previous work, molecular models for 78 real pure fluids were developed, using polar two-center Lennard-Jones potentials [1,2]. Out of more than 3,000 binary mixtures that can be formed from these 78 components, for 354 experimental vapor-liquid equilibria are available in the literature. All these are studied in the present work, so that it is probably the largest systematic study on vapor-liquid equilibria of mixtures with molecular simulation that has ever been carried out.

Vapor-liquid equilibria were calculated in two modes: a) without adjustment of any binary parameters, and b) with adjustment of one state independent binary parameter to one single vapor pressure of a mixture [3,4]. The results are systematically compared to experimental data, as well as to both the empirical Peng-Robinson EOS and the newly developed physically based perturbed-chain polar SAFT (PCP-SAFT) EOS [5,6]. The molecular models yield high quality predictions, and can safely be used in practical applications or in simulative studies where mixture properties are needed, e.g., adsorption processes.

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