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A Monte Carlo Simulation Study of the Liquid–Liquid Equilibria for Binary Dodecane/Ethanol and Ternary Dodecane/Ethanol/Water Mixtures

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Abstract

Obtaining knowledge of the mutual miscibility of alkanes, surfactants, and water over a wide range of temperatures and pressures is of great relevance for the energy industry. Molecular simulations using advanced sampling techniques and transferable force fields can serve as a predictive method to study a variety of phase equilibria at different temperatures, pressures, and overall compositions. In this work, configurational-bias Monte Carlo simulations in the NpT Gibbs ensemble with the Transferable Potentials for Phase Equilibria (TraPPE) force field are applied to investigate the binary mixture of n-dodecane and ethanol at pressures of 0.1 and 100 MPa and the ternary mixture of these compounds with water at one state point. The simulations qualitatively reproduce the increase of the upper critical solution temperature (UCST) with increasing pressure, but the miscibility gap is overestimated at both pressures and the UCSTs are shifted up by about 50 K compared to