Molecular Simulation Approach for Computing Liquid-Vapor Saturation Properties

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The phase behavior of fluids plays an important role in the design of many industrial processes. Here, we describe an approach for computing the phase coexistence properties of complex fluids via reservoir-based grand canonical Monte Carlo simulation. Transition matrix Monte Carlo methods and multicanonical sampling are used to construct a density probability distribution at a temperature of interest, from which saturation properties are deduced. Expanded ensemble techniques are used to gradually insert molecules maintained in a reservoir. Hybrid Monte Carlo moves are used to sample the intramolecular degrees of freedom of a molecule. Finally, we describe a means to efficiently trace the liquid-vapor saturation line via a temperature expanded ensemble. Results will be presented for several industrially-relevant compounds, including octane, cyclohexane, propanol, and squalane.