

## **Molecular Simulation of Vapor-Liquid Equilibria of Highly Associating Systems.**

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Surfactants are industrially important materials because of various applications in the cosmetic, pharmaceutical, and food industries. Ethoxylated alcohol  $\{H-(CH_2)_i-(OCH_2CH_2)_j-OH \text{ or } C_iE_j\}$  surfactants are a particularly interesting class of substances because they have both ether (O) and hydroxyl (OH) groups in the one molecule. For successful usage of these materials in process design and operation, it is essential that phase behaviors for pure and mixtures containing nonionic surfactant systems, such as vapor-liquid equilibria and liquid-liquid equilibria are accurately known. However, few data are available for hydrocarbon + surfactant systems. In the absence of experimental data, empirical correlations and semi-theoretical equations of state are frequently used to predict phase equilibria. However, formulation of these equations requires accurate knowledge of the pure component critical properties and phase behaviors of the constituent molecules. Therefore, it is increasingly important to predict phase equilibria using molecular simulation. Quantitative predictions of phase equilibria from simulation studies are highly dependent on the development of accurate force field models. Unlike the situation for alkanes, studies to estimate the force field parameters for surfactants are limited. In this work, we proposed a new set of force field parameters of surfactants and molecular modeling method bases on atomistic computer simulation were used to estimate thermodynamic properties (densities, critical points, phase equilibria, and so on) of highly associating systems.