Prediction of Limiting Activity Coefficients and Extents of Association using Molecular Modeling and MD Simulation

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The polar and perturbed form of the statistical associating fluid theory (Polar PC-SAFT) was used to model lower 1-alcohol-alkane system. The ability of the equation of state to predict accurate activity coefficients at infinite dilution for 1-alcohol in alkane was demonstrated. Moreover, extents of association are compared to experimental data and MD simulations demonstrating the impact of considering polar interactions. Pure component parameters fitted for alcohols were then extrapolated to approximate pure water SAFT parameters which were validated through predicting the extent of association for the pure component, the solubility and the activity coefficient at infinite dilution for water in alkanes. Results show good agreement with experimental data and MD simulation demonstrating the theory's predictive power as well as the importance of considering polar interactions for better hydrogen bonding thermodynamics.