Molecular Properties of Water/Octane/Ethanol Systems

Joseph R. Michalka and Becky L. Eggimann
Department of Chemistry, Wheaton College, 501 College Ave., Wheaton, IL 60187

Many scientifically interesting processes take place at the interface between immiscible liquids. One such process occurs in the event of a gasoline spill where a hydrophobic fuel phase comes in contact with a hydrophilic water phase in ground water. If the gasoline contains ethanol, many harmful additives and pollutants can find their way into the water table through a co-solvency effect. To begin exploring the microscopic details of this phenomenon, we perform molecular simulations of water/octane systems with ethanol added in three concentrations: 0%, 10% or 25% by volume of the octane phase. We use configurational-bias Monte-Carlo simulations in the isobaric-isothermal Gibbs ensemble to explore structural and thermodynamic properties, including density profiles, radial distribution functions, orientational preferences of water and octane near and far from the interface, interfacial tensions, and solubilities. Two types of simulations were performed: one with water and octane in separate boxes to give bulk liquids in equilibrium, and the other with water and octane in the same box yielding an explicit liquid-liquid interface between equilibrated bulk phases. Each system was started from several different initial configurations where ethanol was placed in the octane, water or interfacial regions and allowed to equilibrate.