Understanding Bulk and Interfacial Properties of Octane-Water-Rock Systems Using Monte Carlo Simulation

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Aqueous hydrocarbon systems are of considerable interest in many applications ranging from the petrochemical industry to biological process and environmental protection. A comprehensive understanding of the phase and interfacial behavior for such systems is important to improve these applications. In the presentation, we first discuss the development of Monte Carlo simulation methods for determining the bulk and interfacial properties of systems that exhibit liquid-liquid phase separation. We present a series of results for a binary Lennard-Jones system that exhibits complex bulk phase behavior. We next show how these approaches are applied to realistic models of water-octane systems in the vicinity of mineral surfaces. For the bulk system, we trace water-rich liquid-vapor (VLE), octane-rich liquid-vapor (VLE), and liquid-liquid (LLE) saturation curves over a wide range of temperatures, pressures and compositions. These curves are constructed via a combination of direct grand canonical simulations and various expanded ensemble schemes. Analogs of these techniques are used to calculate interfacial properties of the water-octane mixture at a silica surface. We present results that show how wetting properties, such as the contact angle of a water droplet at a silica surface in a mother octane phase, evolve with temperature, pressure, and composition.