Understanding the Interfacial Properties of Hydrocarbon-Water-Rock Systems using Molecular Simulation

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Understanding the interfacial properties of the hydrocarbon-water system is important for the design of many industrial applications, including enhanced oil recovery processes. Oil reservoirs consist of porous rock (minerals) in intimate contact with aqueous and oil phases. Reservoirs are often characterized by the phase that has a greater affinity for the rock surface. In the so-called "water-wet" case, water preferentially wets the mineral surface and oil is displaced from the interior of pores. For the "oil-wet" scenario, this relative preference is reversed. From an oil recovery perspective, one generally prefers the water-wet case, as oil is the more mobile phase and is driven to the surface as pressure is applied to the well. Under oil-wet conditions, the water needs to overcome a capillary pressure, which depends on two key interfacial properties: (1) the tension between the hydrocarbon-rich and water-rich phases and (2) the contact angle that a water-rich droplet forms on a mineral surface in a mother alkane-rich background. We discuss here the use of Monte Carlo (MC) molecular simulation to measure these properties for hydrocarbon/water mixtures in the presence of an atomistically detailed mineral surface. We first describe our recent efforts aimed at development of general Monte Carlo simulation methods for determining the wetting properties of fluids at solid surfaces. Our strategy involves calculation of the surface excess free energy (also referred to as the interface potential) as a function of the surface density of a fluid in contact with the substrate at a specified temperature and activity. We then show examples of the application of this general strategy to a model hydrocarbon/water/rock system. Results are presented for the evolution of the contact angle and interfacial tension over a range of pressures and temperatures. We also discuss how polar organic components influence wetting properties. Finally, connections between our results and those from experimental studies are examined.