

# Exploring Lubricants: Investigating the Solid-Liquid Interface Using Molecular Simulation

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Monte Carlo simulations provide an ideal method to examine atomic-scale behavior, such as the interaction of the molecules within a lubricants with a solid surface. In particular, we are interested in competitive adsorption from multicomponent, alkane-rich liquids, as well as the effects of the substrate on molecular orientation within the liquid. Strong evidence of preferential adsorption as a function of strength of attraction with the solid substrate is seen in all simulations. For example, the figures to the right show densities profiles of these two mixtures near the solid substrate. For a strongly interacting ether molecule in an equimolar mixture with a linear alkane of the same length, the ether is the majority species at the interface (left). In the region within six angstroms of the solid, the mole fraction of the ether is 0.99. When the number of interaction sites in the alkane is increased, the composition shifts toward more alkane at the surface. This is evident in mixtures of the same ether with an alkane with a similar total heat of adsorption with the surface. In this case, the mole fraction of the ether within six angstroms of the surface is 0.76 (right).

