468a Monte Carlo Studies of Confined Lubricant Molecules and the Conditions That Lead to Lubrication Failure

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Lubrication failure often occurs where asperities on opposite sliding surfaces come into close proximity. The lubricants which fill the nanometer-scale gaps between asperities can experience high stress and temperature increases of several hundred degrees above the temperature of the bulk. The high temperature and stress may cause lubricant failure due to a combination of mechanical squeezing out and desorption from the surfaces, leaving them susceptible to wear.

Lubricants confined between solid surfaces are studied here using molecular level Monte Carlo simulations with straight chain alkanes as model lubricants. The purpose of this research is to illuminate lubricant behavior in such confined spaces and identify conditions where lubricant failure may occur.

Simulations in the grand canonical ensemble (μ V T) have produced adsorption/desorption isotherms for model lubricant molecules as well as information about the average position and orientation of the molecules in the gap between asperities. Although isotherms for shorter alkanes in slit pores have previously been reported, isotherms at higher temperatures and for chain lengths representative of lubricants have not. Many factors affecting the lubricant behavior have been studied in this work, including lubricant chain length, the distance between the solid surfaces, lubricant pressure and system temperature. The solvation pressure can also be calculated from grand canonical simulations. A plot of the solvation pressure as a function of gap width shows oscillations corresponding to the ordered layering of the molecules.

Simulations in the grand isostress ensemble (μ P_{zz} T) allow Monte Carlo moves which change the gap width during the simulation. With these moves, the equilibrium separation between the solid surfaces is calculated. The pressure pushing the surfaces together (P_{zz}) can be altered to find the point where all of the lubricant is squeezed out of the gap and the solid surfaces come into contact, representative of lubrication failure.