MOLECULAR DYNAMICS SIMULATION OF THE BEHAVIOR OF THIN LUBRICATION FILM

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ABSTRACT

Lubrication system is an essential component for spacecrafts, and lubrication failure has become one of the challenges in developing advanced space technology. However, the process and mechanism of lubrication in space is still unclear due to a complex environment in both physicochemical and mechanical aspects. Molecular dynamics simulations provide new insights to understand the lubrication behavior, especially at the thin film lubrication state. In this work, we study the lubricant conformation changes and energy transfer of confined thin lubricant films by molecular dynamics simulations. It can be concluded that the thickness of film has a power exponential relationship with the pressure loads and the film presents a stratification phenomenon. By introducing the moving slab, the film velocity will redistribute under the entanglement among polymer chains and the friction of the adjacent layers, during which the polymer conformation will change through a "one-step" or "two-step" adjustment. Under low pressure loads, the film behaves like the Couette flow and the temperature profile is parabolic as well as symmetrical, with the maximum temperature appearing at the center of the lubrication film, which may cause the film's viscosity to diminish and ultimately result in lubrication failure. Under high pressure load, the boundary slip phenomenon occurs and the temperature jump exists. From our simulations, it can be noted that the increase in pressure load can lead to a boundary slip phenomenon, where the load-carrying capacity decreases due to the slip and lubrication failure may occur. This work provides new guidance in understanding the lubrication behavior in space.