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Molecular mobility analysis to explain lubricated friction at high pressure

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This work provides insights for friction prediction in elastohydrodynamic lubricated contacts under high pressure. From Equilibrium Molecular Dynamics simulations, diffusion coefficient and relaxation time for Squalane and Benzyl Benzoate are obtained on a wide range of pressure and temperature. Newtonian viscosity is derived through a Stokes-Einstein relation and successfully compared with experimental measurements from viscometers. Discussion is then undertaken to link relaxation time with a fluid critical shear rate. Friction prediction at high pressure and shear can be obtained via a stress augmented activation energy model, able to capture situations close to "limiting shear stress" as seen in friction experiments.

Keywords: Molecular dynamics, EHL, friction

1. Introduction

Under severe conditions (such as high pressure), friction in elastohydrodynamic regime may exhibit an apparent plateau regime, where friction becomes nearly independent on sliding velocity.

Up to now, there is no common consensus on the physics at stake that would explain such "solid-friction-like" behavior. In-situ measurement methods are not yet available to study local phenomena in these severe conditions. Molecular Dynamics simulations were used by Ewen et al. [1] who suggest that this so-called limiting stress would be a signature of the molecular structure of the lubricant involved. On the other hand, Porras-Vazquez et al. [2] showed that whatever the fluid, the physical state imposed by the thermodynamic conditions would be the key to this phenomenon. To go deeper into this investigation, Molecular Dynamics simulations are here used to probe molecular mobility.

2. Methods

Two fluids of different nature are selected: Squalane (noted SQ, an elongated alkane typical of classical base oils) and Benzyl Benzoate (noted BB, a bulky molecule akin to traction fluids). Mean Square Displacement from Equilibrium Molecular Dynamics (EMD) simulations are used to compute the diffusion coefficient over a large range of pressure, temperature, and shear rate.

As described in Figure 1 for SQ (the same kind of result is also obtained for BB), the diffusion coefficient follows an Arrhenius law, whose activation energy is proportional to pressure.

Relaxation time as well as Newtonian viscosity (Stokes-Einstein relation) are then derived from the diffusion coefficient.

3. Discussion

We assume that the relaxation time is inversely proportional to a critical shear rate that the fluid would be able to undergo in a purely liquid state. From this, one would explain the viscosity (and thus friction) change under high pressure with a drastic change of relaxation time and thus of Weissenberg number (Wi = effective shear rate times relaxation time).

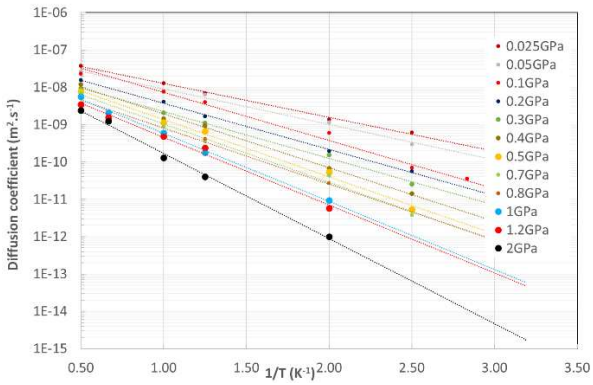

Figure 1: Diffusion coefficient for squalene obtained with EMD.

Jadhao and Robbins [3] showed that SQ viscosity follows an Eyring law over a wide range of Wi. Interestingly, this law based on the concept of stress augmented activation energy is a perfect relay between EMD investigation able to probe Newtonian viscosity and relaxation time (both functions of pressure and temperature), and friction prediction at high shear rate (non-equilibrium).

For Wi of the order of 10^5, the Eyring normalized viscosity (NV: effective viscosity divided by Newtonian viscosity) evolves as $Wi^{-0.91}$, suggesting that friction experiment could experience an apparent limiting shear stress.

4. References

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