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ATOMIC-SCALE MODELLING OF LUBRICANTS AT HIGH PRESSURE: ON THE COMPETITION OF SHEAR THINNING, THERMAL THINNING AND WALL SLIP

M. Moseler*, S. Peeters, L. Kruse, F. Stief, E.Garcia, H. Holey, T. Reichenbach, G. Moras, K. Falk
*Michael.Moseler@iwm.fraunhofer.de
Fraunhofer IWM, Mikrotribologie Centrum µTC, Wöhlerstr. 11, 79108 Freiburg, Germany

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ABSTRACT

Modern, compact and efficient tribological systems are often operated in mixed lubrication or even boundary lubrication. This means small gaps, frequently high pressures and occasional solid-solid contacts between the lubricated sliding surfaces. In particular, the need for climate-friendly lubricants with low viscosities, an increase in assembly precision of lubricated contacts for electric vehicles and new high-performance coatings that allow smaller assembly tolerances have driven the shift to operating devices in the mixed and boundary lubrication regime. A fundamental understanding of the rheological properties of lubricants in narrow gaps under high pressures and elevated temperatures is mandatory for a predictive modelling as well as a knowledge-based design of boundary-lubricated devices. Especially, the identification of the relevant velocity accommodation mode is a challenging task, since it results from an intimate interplay of pressure-induced viscosity increases, temperature-induced and shear-induced viscosity decreases as well as shear-induced wall slip. Molecular dynamics simulations are ideally suited to study and shed light into the balance of these different mechanisms [1]. Fortunately, recent developments in force fields allow for faithful atomistic models with steadily increasing complexity [2].

This presentation reports our activities for the predictive modelling of the high-pressure rheology of mineral oils [3] and water-bases lubricants – including the calculation of viscosities at high pressures [4] and shear rates as well as wall slip [5] under extreme confinement and pressures [1]. These results are useful for a subsequent continuum description of boundary lubricated contacts. Continuum theories using for instance the Reynolds Lubrication Equation (RLE) are expected to fail for lubricant film heights $h_0 \ll 10\ nm$, especially in highly loaded tribosystems with normal pressures $p_n \gg 0.1\ G\text{Pa}$. Here, the performance of RLEs is validated by molecular dynamics sliding simulations of pressurized (with $p_n = 0.1 - 1$ GPa) hydrocarbon lubricants in a converging-diverging channels with minimum gap heights $h_0 = 1.4 - 10$ nm (Fig. 1). For $p_n \leq 0.4$ GPa and $h_0 \geq 5$ nm, agreement with the RLE only requires accurate constitutive laws for pressure-dependent density and viscosity. An additional non-linear wall-slip law extends the RLE's validity to even the most severe loading condition $p_n = 1$ GPa and $h_0 \approx 1$ nm (compare black and red curves in Fig. 1) Our results demonstrate a novel route for non-empirical predictive continuum modelling of boundary lubrication.

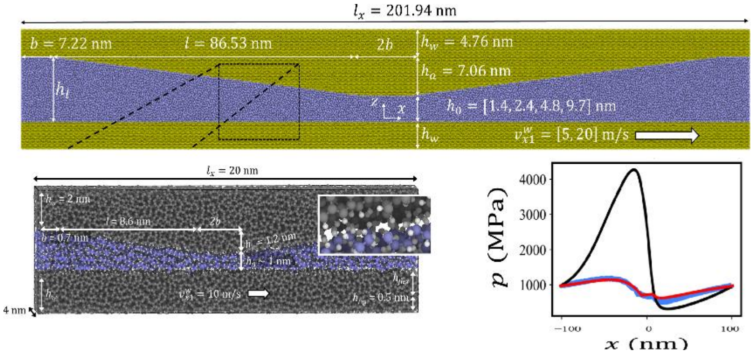

Fig. 1: Converging-diverging channels of gold and DLC filled with hexadecane and PAO4, respectively. Bottom right panel: pressure along the $\boldsymbol{p_n} = \mathbf{1\ GPa}$ and $\boldsymbol{h_0} \approx \mathbf{1\ nm}$ gold channel (blue: molecular dynamics, black: Reynolds with no slip, red: Reynolds considering slip).

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