Constitutive modelling of lubricants with optimized-potential molecular simulations

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Motivation

Friction and wear are one of the most fundamental sources of world-wide energy loss. Besides the direct environmental impact (e.g. CO2 emission, irrecoverable material losses) there is also a clear economical cost. Adequate lubrication is crucial to minimize friction and wear, assuring optimal energetic performance, durability, reliability, and finally a guaranteed expected lifetime of machine components.

Bearings and gears are two of the most common components in mechanical equipment. These components operate ideally under the so-called **Thermo-Elastohydrodynamic Lubrication (TEHL) regime** where the surfaces that are in relative motion are completely separated by a thin lubricant film (< 1 µm). In this specific regime, the lubricant film experiences high hydrodynamic pressures (up to 4 GPa) resulting in elastic deformation of the surfaces. Apart from the high pressures, very high shear rates (> 10^8 s^{-1}) and high contact temperatures may occur, depending on the slide-to roll ratio of the contact. It is widely known that **in TEHL, thermomechanical properties of the lubricants are heavily influenced by the pressure, shear rate and temperature due to the supposed intensified interaction between the lubricant molecules**, leading to compressible, piezoviscous and Non-Newtonian behaviour.

As it is very difficult to perform experiments at ultra-high pressures in combination with high shear rates representative for TEHL contacts, in the recent decade, there has been an exponential increase in the use of **Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations** for the investigation of complex nanoscale behaviour and the identification of thermomechanical properties of lubricants in TEHL. While equilibrium MD (EMD) simulations are suited to study lubricant properties at low shear rates, **non-equilibrium MD (NEMD) simulations** are of particular interest to study non-Newtonian lubricant behavior at high shear rates that are relevant for TEHL.

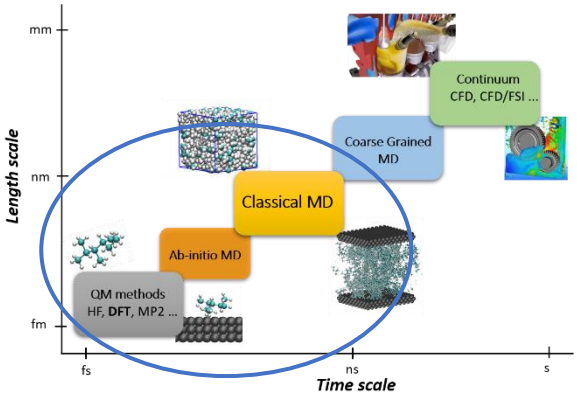

Figure 1 All accessible scales of computer modelling methods for tribological system and scale of interest of the current project.

Objectives

In the context above, Soete Laboratory and the Center for Molecular Modelling at UGent team up and combine their complementary expertise. **The global objective is to map all relevant thermomechanical properties of a well-defined lubricant as a function of** three state variables namely **pressure, temperature and shear rate, in the ranges relevant for TEHL by using NEMD simulations**.

To achieve this goal, we first aim to develop **reliable and accurate force field models from dispersion-corrected**

Density Functional Theory (DFT-D) simulations to describe intra- and inter-molecular interactions within lubricated contacts as the existing force fields in literature do not capture these properties under such extreme conditions of TEHL. The developed model will be used to study thermomechanical properties of lubricants under TEHL conditions.

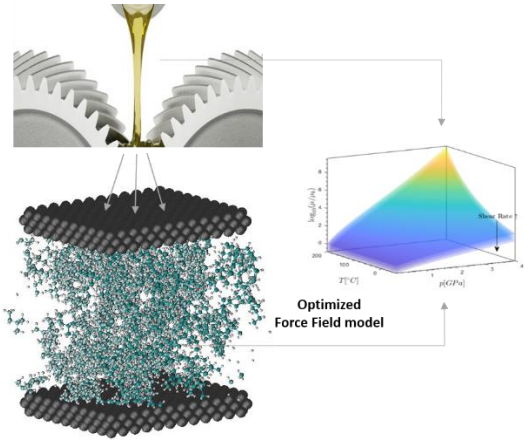

Figure 2 A representative figure describing the ultimate goal of the project.

APPROACH

To accomplish the objectives, a comprehensive atomic-scale investigation will be carried out starting from DFT-D calculations of lubricant molecules and iron oxide lattices, which are formed at steel surfaces when they exposed to air. The DFT-D calculations involve (i) interactions between lubricant molecules/conformational barriers, (ii) interaction within the iron-oxide surface, (iii) the interfacial interaction between lubricant molecules and iron oxide surfaces (i.e. adsorption characteristics).

The generated database from DFT-D calculations will be used to optimize force fields with improved accuracies to be used in subsequent MD simulations. Both bonded and non-bonded terms in the conventional force fields will be refined and optimized from the obtained DFT-D results. In particular, the focus will be on the optimization of the non-bonded interactions to make this optimized force field suitable for ultra-high pressure conditions.

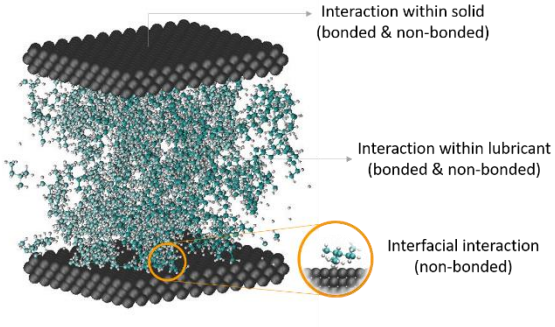

Figure 3 The relevant bonded and non-bonded interactions for lubricated.

The optimized force field will be applied in subsequent NEMD calculations. It is expected that it will significantly improve the predictions of the thermomechanical properties of lubricants that are pertained to TEHL in NEMD simulations. In addition to density and shear viscosity, we also aim to determine bulk viscosity (which is an important property for compressible fluids), thermal conductivity, heat capacity and the limiting wall shear stress from MD calculations.

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