Modelling lubrication at the nanoscale

A multiscale framework for lubrication modelling

Lubricant: mixture of n-hexadecane and ZDDP

- United Atom (CH$_2$ and CH$_3$ groups are considered as one interaction site)
- OPLS force field: considering inter and intramolecular interactions
- Intermolecular interactions: Lennard-Jones and Coulomb

The story

Molecular Dynamics simulations are used to study the tribological performance of a lubricant mixture containing hexadecane base oil and 5% Zinc Dithiophosphate (ZDDP) under molecular confinement conditions. The influence of ZDDP additive on the interfacial response is studied in detail. Simulations demonstrate the migration of ZDDP molecules and their adsorption onto the solid surface resulting in a remarkable suppression of wall slip compared to pure hexadecane. Consequently, the effective shear rate is higher and so is friction.

Reference

Tribology International, 43 (10), 2010, pp. 1811-1822

Effect on wall slip and friction

- With ZDDP adsorbed on iron oxide surfaces, wall slip is greatly reduced.
- The effective shear rate $\dot{\gamma}$ of the lubricant significantly increases.
- As a result, shear stress $\tau_{xz}$ representing friction, also increases.

<table>
<thead>
<tr>
<th>Film composition</th>
<th>$\dot{\gamma}$ ($x 10^9$ s$^{-1}$)</th>
<th>$\tau_{xz}$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100% n-hexadecane</td>
<td>4.30</td>
<td>93.6</td>
</tr>
<tr>
<td>95% n-hexadecane+5% C4-ZDDP</td>
<td>8.26</td>
<td>115.7</td>
</tr>
</tbody>
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This friction increase caused by ZDDP addition is in accordance with reported experimental findings. MD simulations propose an explanation of this phenomena.