Thermophysical Properties of Lubricants at Extreme Conditions: Experiments, Molecular Simulation and Modeling

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Lubricated contacts between machine elements are subject to extreme pressures up to 4 GPa. For modelling tribo-contacts on the macroscale, reliable models of the thermophysical properties of the lubricant fluids are required. At such conditions, thermophysical properties of lubricants are difficult to measure. In this work, a variety of model lubricants were studied, including squalane, 1-octanol, and 1-hexadecane, by combining experiments, molecular dynamics simulation, and molecular-based equations of state. In a first step, molecular dynamics simulations were used for determining the most accurate and reliable transferable force field for modelling branched alkanes [1], which turned out to be the Potoff united-atom force field. It describes the experimental data (which are generally available only at moderate conditions) often within the experimental uncertainties. Additionally, high-pressure experiments were carried out for determining the viscosity and density of the model lubricants at pressures up to 1 GPa for the viscosity and up to 200 MPa for the density at temperatures in the range of 298–373 K. The hybrid data set of experimental data and molecular simulation data was used for parameterizing a molecular-based equation of state model based on the SAFT-VR Mie equation. For modelling the viscosity, entropy scaling was used. The model describes the hybrid data set very well. It is shown that the obtained model behaves well upon extrapolation to extreme pressures and temperatures. Finally, the applicability of the model in macroscopic tribological simulations is demonstrated [2].

References

1. Schmitt et al., J. Chem. Phys. B. 127, 8 (2023) 1789-1802.
2. Wingertszahn et al., Trib. & Schmierungstech. 70, 4 (2023) 5-12.
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