THERMOPHYSICAL PROPERTIES AT EXTREME CONDITIONS

Dennis Alt, Sebastian Schmitt, Hans Hasse, Simon Stephan*
Laboratory of Engineering Thermodynamics (LTD), RPTU Kaiserslautern, Germany
*simon.stephan@rptu.de

ABSTRACT

Lubricated contacts between machine elements are subject to extreme pressures of up to 4 GPa. To model tribo-contacts at the macroscale, reliable models of the thermophysical properties of the lubricant fluids are required. The density and the viscosity are of particular significance. At such conditions, thermophysical properties of lubricants are challenging to measure experimentally. In this work, a variety of model lubricants were studied, including n-alkanes, squalane, and 1-octanol by combining experiments, molecular dynamics simulation, and molecular-based models. In a first step, 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 120 MPa for the density and in the temperature range 298 – 373 K. Molecular dynamics simulations were used to identify the most accurate and reliable transferable force field for modelling branched alkanes [1], which turned out to be the Potoff united-atom force field. This force field evaluation was carried out by comparing MD predictions to available experimental data. Then, molecular dynamics simulations based on the Potoff force field were carried out for predicting thermophysical properties at extreme conditions, where no experimental data were available. The hybrid data set, comprising both experimental and molecular simulation data, was used for the parameterisation of a molecular-based equation of state model, based on the SAFT-VR Mie equation. For modeling transport properties, such as the viscosity and thermal conductivity, entropy scaling [2] was used. The model describes the hybrid data set very well. The model's performance is further demonstrated by its ability to extrapolate well to extreme pressures and temperatures, as well as mixtures. Finally, the model was used for describing thermophysical properties in tribological elastohydrodynamic simulations [3].

REFERENCES

[1] S. Schmitt et al., Comparison of Force Fields for the Prediction of Thermophysical Properties of Long Linear and Branched Alkanes, *J. Chem. Phys. B.,* vol. 127 (8), pp. 1789-1802 (2023).
[2] S. Schmitt et al., Entropy scaling framework for transport properties using molecular-based equations of state, *J. Mol. Liq.,* vol. 395, pp. 123811 (2024).
[3] P. Wingertszahn et al., Measurement, Modelling, and Application of Lubricant Properties at Extreme Pressures, *Tribol. Schmier.,* vol. 70, pp. 5-12 (2023).