COUPLING MOLECULAR THERMODYNAMICS MODELS WITH CFD SIMULATION ENGINES

Xueqi Zhang[1], Thomas Reviol[2], Jens Staubach[1], Simon Stephan[1,*]

[1]Molecular Thermodynamics Group (MTG), RPTU Kaiserslautern, Germany
[2]Laboratory of Reaction and Fluid Process Engineering (LRF), RPTU Kaiserslautern, Germany
[*]simon.stephan@rptu.de

ABSTRACT

Analytical molecular thermodynamics models are an attractive option for the modeling of thermophysical properties of fluids. The basis of this model class are molecular-based equations of state, e.g. PC-SAFT [1] or SAFT-VR Mie [2]. These models enable the description of static properties. For describing intramolecular thermodynamic properties, a quantum mechanical model is used. Using auxiliary models such as density gradient theory and entropy scaling [3], also interfacial and transport properties, respectively, can be described. These models can be used even when very limited data are available and can be used for extrapolation of extreme conditions. In particular, they can be applied for predicting mixture properties based on the pure component models alone. We have developed a software package, called MicTherm, that contains a large library of such molecular thermodynamics models. MicTherm comprises an application programming interface (API) for the coupling to other simulation engines – especially Computational Fluid Dynamics (CFD) simulation packages. A schematic representation of the coupling is shown in Figure 1. CFD simulations typically require the specification of several thermodynamic properties, such as the viscosity, thermal conductivity, phase equilibrium properties, heat capacity, speed of sound and density at a given temperature and pressure and eventually composition if mixtures are considered. In CFD simulations, traditionally very simple models for the thermodynamic properties are employed, e.g. the ideal gas model or a constant density model. However, fluid properties play a crucial role in ensuring accurate simulation outcomes. We demonstrate the feasibility of coupling MicTherm with CFD simulations by using OpenFOAM. Also, results are presented for coupling MicTherm with elastohydrodynamic fluid simulations [4]. This general concept can be used for various CFD engines for the modeling of various thermophysical fluid properties. This enables the modeling of thermodynamic properties and transport properties using thermodynamically consistent frameworks that are applicable also in metastable states, across large ranges of pressures and temperatures, for mixtures, and phase equilibria.

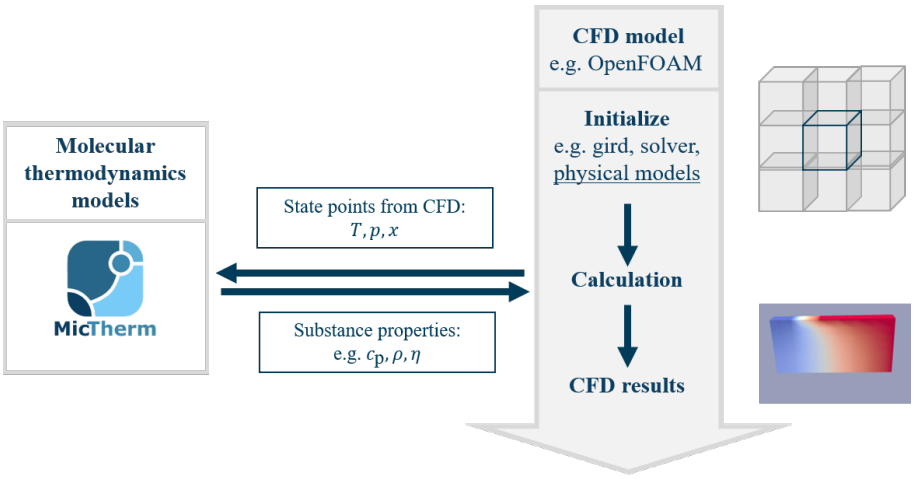

Figure 1: Schematic representation of the coupling of molecular themrodynamics models with CFD simulation engines.

REFERENCES

[1] T. Lafitte et al., Accurate statistical associating fluid theory for chain molecules formed from Mie segments, *J. Chem. Phys.*, vol. 139, pp. 154504, 2013.
[2] V. Papaioannou et al., Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments, *J. Chem. Phys.*, vol. 140, pp. 054107, 2014.
[3] S. Schmitt et al., Entropy scaling framework for transport properties using molecular-based equations of state, *J. Mol. Liq.*, vol. 395, pp. 123811, 2024.
[4] P. Wingertszahn et al., Measurement, Modelling, and Application of Lubricant Properties at Extreme Pressures, *Tribologie und Schmierungstechnik*, vol. 70, pp. 5-12, 2023.