Coupling the molecular thermodynamics software MicTherm with the OpenFOAM CFD simulation engine

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Introduction

MicTherm is a software package for the modeling of thermophysical property data of fluids and fluid mixtures using molecular thermodynamic models. It contains several molecular-based equation of state (EOS) models for describing static properties as well as auxiliary models for describing transport and interfacial properties. The models included in MicTherm are physical models that often enable extrapolations to regions where no or little experimental data are available.

MicTherm comprises an application programming interface (API) [1] for the coupling to other simulation engines. Here we demonstrate the feasibility of this coupling by using MicTherm in OpenFoam [2] to model the thermophysical properties of a fluid.

Website and Overview

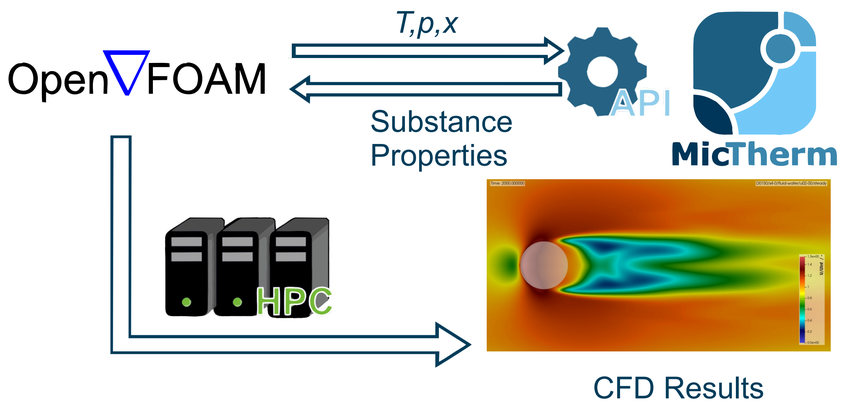


Fig. 1: Schematic representation of the interaction between OpenFOAM and MicTherm.

Workflow

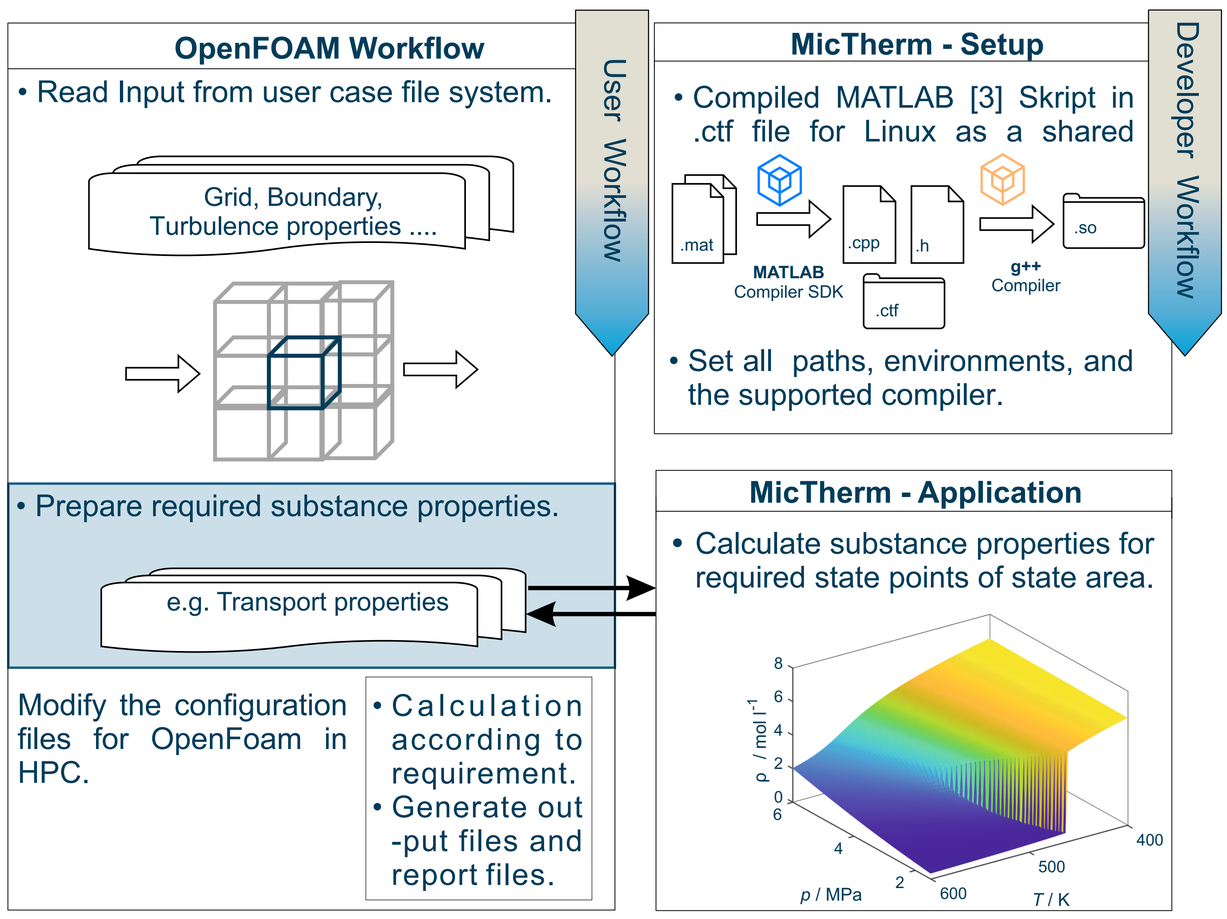
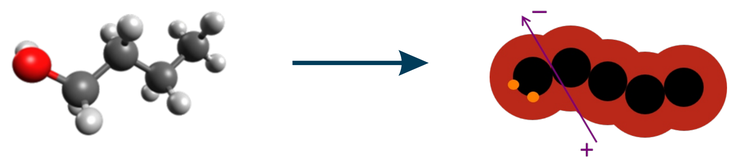


Fig. 2: Workflow illustrating the interaction between OpenFOAM and MicTherm from the user (left) and developer(right) pespectives.

Modeling

The molecular-based EOS can calculate all thermodynamic properties from the Helmholtz energy *a*.

$$a = a^{\text{ideal gas}} + a^{\text{hardsphere}} + a^{\text{monomer}} + a^{\text{chain}} + a^{\text{assoc}} + a^{\text{polar}}$$



- Derived from molecular properties of pure substances and mixtures.
- Covers homogeneous states and phase equilibria.
- Utilizes about 10 substance-specific parameters.
- Enables fast calculation of extensive thermodynamic properties.
- Robust extrapolation behavior.

Available Thermophysical Properties

MicTherm contains only fundamental EOS, i.e. models formulated in the Helmholtz energy such that all static thermodynamic properties can be calculated from a given EOS, e.g. speed of sound, pressure, heat capacity, compressibility, enthalpy of vaporization, vapor pressure, etc. For modeling interfacial properties, e.g. surface tension, the density gradient theory [4,5] is implemented in MicTherm. For modelling transport properties, such as viscosity and thermal conductivity, entropy scaling [6] and friction theory [7] are implemented in MicTherm.

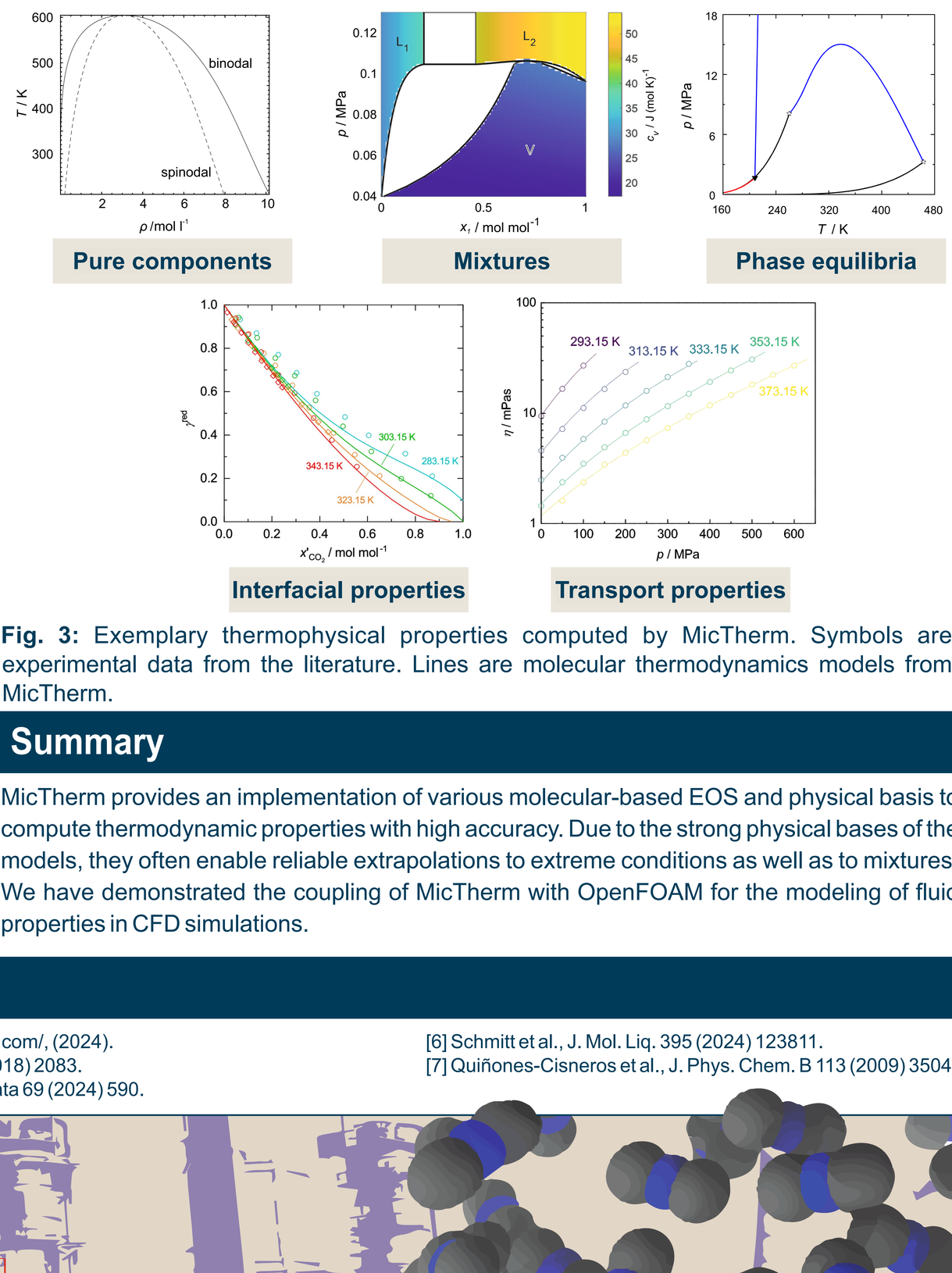


Fig. 3: Exemplary thermophysical properties computed by MicTherm. Symbols are experimental data from the literature. Lines are molecular thermodynamics models from MicTherm.

Summary

MicTherm provides an implementation of various molecular-based EOS and physical basis to compute thermodynamic properties with high accuracy. Due to the strong physical bases of the models, they often enable reliable extrapolations to extreme conditions as well as to mixtures. We have demonstrated the coupling of MicTherm with OpenFOAM for the modeling of fluid properties in CFD simulations.

Literature

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