University of Stuttgart
Germany

SUPER – Stuttgart University Program for Experiencing Research
Project Information

Institute's Information

Name of Institute	Institute of Thermodynamics and Thermal Process Engineering ITT
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Duration of Project/Number of Students

June/July	x
June/July/August	x (both)
Number of Students	1

Name of Project Determining thermodynamic properties with molecular models

Beneficial Skills & Knowledge

Basics in Thermodynamics and numerical methods

Prior knowledge in programming (Python) helpful but not required

Description of Work

For apparatus and process design knowledge of the thermodynamic properties (for example the boiling point, density, vapour-liquid-equilibrium, thermal conductivity, viscosity, ...) of a working fluid is important. Depending on the substance and property the prediction of these properties can be challenging.

In thermodynamics we have several methods to predict substance properties such as molecular simulations, equations of state, density functional theory, machine learning methods and more. You can find a brief overview of our general research topics at:
https://www.itt.uni-stuttgart.de/en/research/

To give you an idea what a specific topic would look like you can see an exemplary project from our research area "Simultaneous process and solvent design":

Determining the viscosity of mixtures with entropy scaling

Transport properties (for example viscosity or thermal conductivity) of a working fluid can be very difficult to predict because they display a very complex behavior over for example temperature and pressure.

As mentioned before, we have several methods to predict these properties. The method you will use is called entropy scaling. In the residual entropy space, transport coefficients can be predicted fairly simple and with good accuracy because we observe a univariate behavior. For mixtures, we need the so called mixing rules that enable to predict mixture properties from pure substance data. Your job would be to optimize the mixing rules to best represent the mixture data, based on the residual entropy space.

We use the programming language Python via Anaconda for most of our work, so you would implement and test the mixing rules in this programming environment. This helps the research to be reproducible and for data to be used later for deep learning and/or machine learning models.

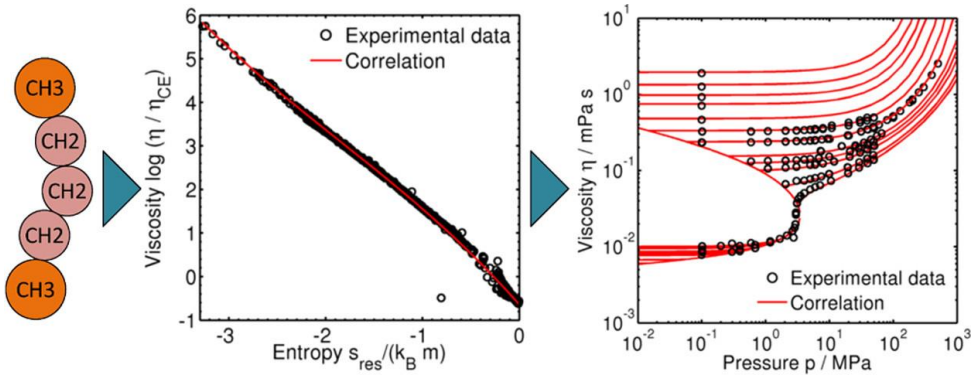

Figure 1: Here is how we can represent the viscosity in the residual entropy space. Values for different temperatures and pressures fall into an almost straight line, while if we have pressure on the x-axis, the behavior is much harder to describe. Viscosity prediction with Entropy Scaling (Lötgering-Lin et al. 2015)

We will determine your research question together, depending on your interest, the available topics and the state of the research when you arrive. As research progresses fast we can't guarantee that every field of research will have a topic available.