Thesis type: Master thesis

Starting date: ab 06.11.2018

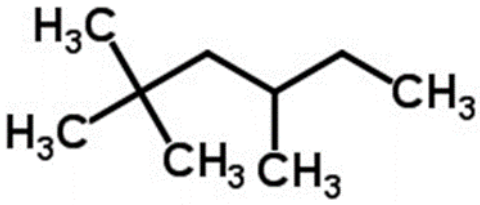
Fully Predictive Equation of State for Viscosity Prediction of Normal and Branched Alkanes

Our profile:

In the research group “Model-based Fuel Design” at Institute of Technical Thermodynamics or Lehrstuhl für Technische Thermodynamik (LTT), we developed a fully predictive model of an equation of state based on Perturbed-Chain Polar Statistical Associating Fluid Theory (PCP-SAFT). The development has implemented prediction of phase-change thermodynamics data, such as vapor pressure, liquid density, and enthalpy of vaporization.

Your tasks:

Currently, we are developing our predictive model to also include viscosity prediction. The viscosity prediction will be based on the entropy scaling theory which has been evaluated on group-contribution method for PCP-SAFT in literature. Instead of using group contribution method, your task is to develop a model for directly estimating entropy scaling coefficients based on molecular descriptors. The molecular descriptors can be based on molecular structure or be derived from quantum mechanical calculations. Some molecular descriptors have been introduced in our last development of fully predictive PCP-SAFT. As part of this master’s thesis, you must investigate the correlation between the molecular descriptors and the entropy scaling coefficients. If needed, some new molecular descriptors may need to be introduced. The model must be evaluated for normal and branched alkanes.



2,2,4-trimethylhexane, an example of branched alkanes

Our offer:

Write your master thesis with excellent supervision in a motivated team. You get an insight into scientific working methods and deepen your knowledge in programming and theories of thermophysical properties. There is also the possibility of a publication.

Your profile:

Ideally, if you are interested in physical chemistry, programming (Python or others), and correlation analysis, then we would like to get to know you better in our team.

Please don’t hesitate to write us an email to the following address:

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