Investigation of the applicability of a predictive equation of state to model multi component mixtures

Keywords
Thermodynamics of mixtures, Molecular Thermodynamics, Equations of State, Quantum Mechanics

Our Profile
The Chair of Technical Thermodynamics (LTT) at RWTH Aachen investigates questions of energy and chemical engineering along the entire “thermodynamic elevator”: This ranges from the structure and properties of individual molecules, over the analysis of a single process towards the evaluation of entire energy systems. The group molecular systems engineering at the LTT explores the behaviour and properties of fluid and solid substances depending on their molecular structure and interactions.

Background
For sustainable Processes it is necessary to replace fossil resources with biomass as a carbon source. A Problem of biomass as a carbon source are the high energy costs of the resulting processes that are caused primarily by the separation of water. High Pressure Switchable Water (HPSW) is a promising method to separate water and organic compounds efficiently[1].

Assignment
Our group has developed a model that allows the prediction the PCP-SAFT[2] Equation of State (EOS) parameters for arbitrary molecules. You will use an existing implementation of the PCP-SAFT EOS[2] and the SEPP[3] Model for the parameter prediction to determine thermodynamic properties (e.g. phase equilibria) for several molecular systems. The focus will be on systems that are used in the HPSW method, i.e. mixtures containing water, CO\textsubscript{2}, amines and organic compounds (e.g. acetone). The goal of the thesis is to evaluate the applicability of the PCP-SAFT EOS as well as other property models (e.g. COSMO-RS) on these systems, and to identify possible problems and improvements. Depending on the extend of the thesis further evaluation with other extensions of the SAFT EOS (e.g. e-PC-SAFT) can also be considered.

Your Profile
You study Maschinenbau/Wirt.-Ing. MB/CES with specialization in chemical or energy engineering or something comparable. You are interested in current research topics concerning thermodynamics and chemical engineering you are proficient in thermodynamics of mixtures or molecular thermodynamics. Previous experience in Python, Java or a comparable programming language are of advantage but not absolutely necessary. The same applies for experience with the “RWTH Compute Cluster”. You can work on complex assignments individually and target oriented.
Our Offer

You work in a young, motivated team on solving a current research question. In addition you can expand your knowledge in the area of thermodynamics, programming and parallel computation. This thesis does not require any experiments, therefore it is possible to complete the entire thesis from your house. You will have the possibility of frequent exchange with your supervisors via online meetings. Also in case of a situation where the current state of the Covid-Pandemic no longer requires you to work from home office it will be your choice where you want to complete your work. If you are interested you are welcome to contact us via E-mail. (Please append your CV and current overview of grades)