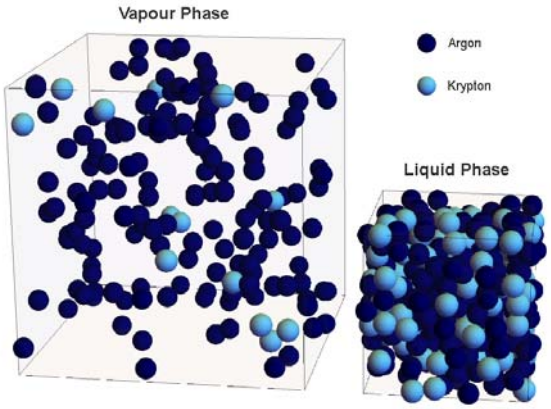
Graz University of Technology
Institute of Chemical Engineering and Environmental Technology
Plant and Process Design & Chemical Engineering Thermodynamics

☒ Bachelor's thesis
☐ Plant design exercise
☐ Paid master's thesis

☒ Computational
☐ Experimental
☐ Plant design related

Molecular Monte-Carlo Simulations

The goal of this research topic, which provides several successive theses, is the application of a continuously developed molecular simulation program that has been realized as a Wolfram Mathematica notebook [1]. This implementation provides a so-called "Continuous Fractional Component Gibbs Ensemble" (CFCGE) Monte-Carlo (MC) simulation environment that is predestined for the determination of phase equilibria. The notebook shall be applied, e.g., to simulate different equilibria (VLE, GLE, LLE), to assess various force fields for different substances, or to explore and optimize simulation strategies. This is done in each case by comparing the simulation results with data from literature and/or equations of state.



A basic knowledge of Wolfram Mathematica concepts is required, e..g. by exploring the interactive site http://www.wolfram.com/wolfram-u/an-elementary-introduction-to-the-wolfram-language/

The thesis can be written in either *English* or *German* and can be done entirely from the home office.

Contact: Assoc.Prof. Dipl.-Ing. Dr.techn. Thomas Wallek
Tel.: +43 (0)316 873-7966
thomas.wallek@TUGraz.at

Start: Continuously

Literature: [1] Mayr N: Improvement of the Molecule Exchange Efficiency in Gibbs-ensemble Monte-Carlo Simulations. MSc-thesis, 2021.