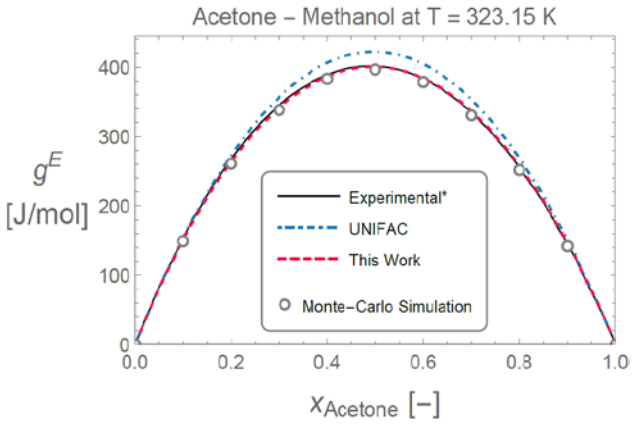
Graz University of Technology
**Institute of Chemical Engineering and Environmental Technology**
Process technology & chemical engineering thermodynamics

☒ Bachelor's thesis
☒ Plant design exercise
☒ Paid master's thesis
☒ Computational
☐ Experimental
☐ Plant design related

## Assessment of activity coefficient models

The goal of this topic is the assessment of a predictive thermodynamic model for the excess Gibbs energy ($g^E$) resp. activity coefficients, which is based on a recently published modeling approach [1]. This is to be done by comparing its results with experimental data from a benchmark database [2] and results from other, established models, like UNIFAC. For this purpose, two-component mixtures of different complexity are investigated, ranging from simple, non-polar molecules to more complex, strongly polar substances. The results of this assessment will be used as a feedback for further improvement of the modeling approach. All relevant models are available as Wolfram Mathematica notebooks, which requires a basic familiarity with the Wolfram Language concepts, e.g., by exploring the interactive introduction http://www.wolfram.com/wolfram-u/an-elementary-introduction-to-the-wolfram-language/. The thesis can be done entirely from the home office and can be written in either English or German.




**Contact:** Dipl.-Ing. Christoph Mayer, BSc
Tel.: +43 (0)316 873-4986
cmayer@tugraz.at

**Start:** February 2022

**Literature:** [1] Mayer C, Wallek T, 2020, https://doi.org/10.3390/e22101111

[2] Jaubert JN et al., 2020, https://doi.org/10.1021/acs.iecr.0c01734

Austrian Science Fund (FWF): P 32609-N