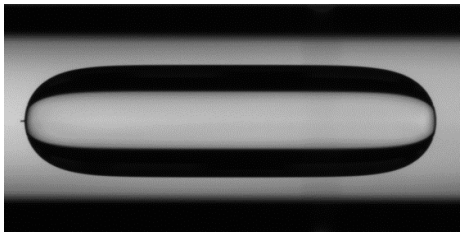
Graz University of Technology
Institute of Chemical Engineering and Environmental Technology

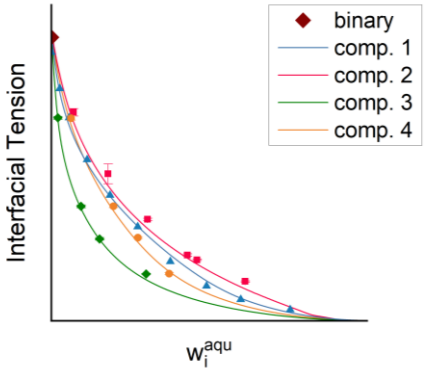
☒ Bachelor Thesis
☒ Plant Design Practice (KÜ)
☒ Master Thesis

☒ theoretical
☐ experimental
☐ constructive

Topic: **Interfacial Properties at elevated Pressure**

The fundamental comprehension of interfacial properties is of decisive importance for the downstream processing of many chemical and pharmaceutical products. In addition to conventional processes, extraction with high-pressure solvents, such as supercritical CO_2, have recently gained attention in industrial applications. For the design and optimization of such processes, the simulation of phase equilibria and interfacial properties of high-pressure systems is imperative.





Within the scope of this project an existing framework for the calculation of phase properties based on the PC-SAFT equation of state (EoS) should be extended to accommodate the calculation of high-pressure phase equilibria and interfacial properties. Moreover, dynamic simulations of the mass transfer through the interfacial boundary should be conducted to predict the net mass flux between the phases during extraction. For that purpose, an existing dynamic model [1] can be coupled with the PC-SAFT EoS.

Contact: Dipl.-Ing. Roland Nagl
nagl@tugraz.at

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Literature: [1] Nagl, R., Zimmermann, P., Zeiner, T., J. Chem. Eng. Data 2020, 65, 328–336.

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