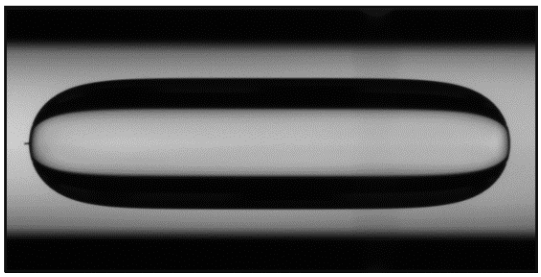
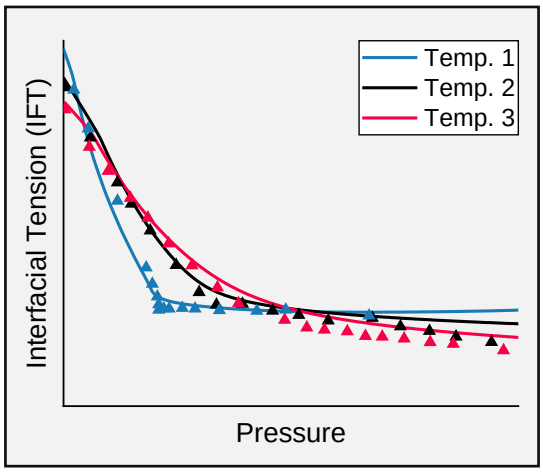
Interfacial Properties at elevated Pressure

Topic suitable for Master Thesis / Bachelor Thesis / Plant Design

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 thermodynamic 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 such as **interfacial tension**. Moreover, dynamic simulations of the **mass transfer** through the interfacial boundary are conducted to predict the net mass flux between the phases during extraction. For that purpose, an existing dynamic model [1], implemented in C++, is coupled with the PC-SAFT EoS.





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Starting date: Upon agreement
Literature: [1] Nagl, R., Zimmermann, P., Zeiner, T., J. Chem. Eng. Data 2020, 65, 328–336. https://doi.org/10.1021/acs.jced.9b00672

FWF Der Wissenschaftsfonds.