Thermodynamics of non-ideal systems at supercritical conditions

High pressure phase behaviour of ternary systems containing CO_2 and two components with different functional groups

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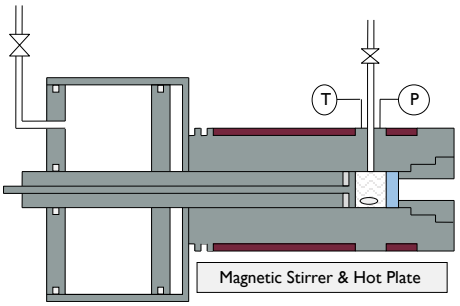
Background

Supercritical CO_2 is an attractive alternative solvent for the processing of high molecular mass compounds due to its generally 'green' and the fact it is a *Generally Regarded as Safe* solvent. However, due to the high pressures and liquid-liquid nature of CO_2 at these conditions, it is very difficult to design and model such processes, hampering development and leading to expensive and time-consuming piloting studies. A need therefore exists for an improved understanding of the underlying fundamentals of such processes.

This larger project will consider the thermodynamics of underlying supercritical CO_2 processes. There already exists information on the phase behaviour of CO_2 + alkanes + molecules with functional groups and this data can be used to describe the interaction between alkanes and the functional group. However, data is as yet not available for ternary systems containing CO2 + two components with differing functional groups. Additionally, due to the lack of data these types of systems have to date not been modelled extensively.

Experimental measurements

- High pressure phase behaviour

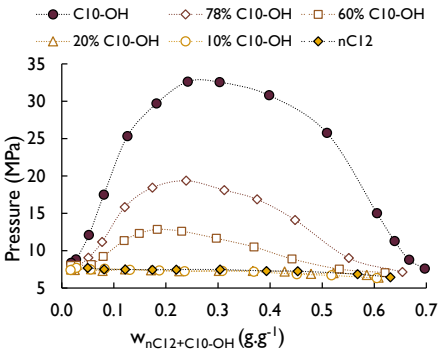


Thermodynamic modelling

- State of the art models vs. models in process simulators

Process Simulation

- Ability to model supercritical fraction processes



Improved understanding of interactions between molecules, prediction of molecular interactions, and the influence of the interactions on phase behaviour and separation ability

Projects available in 2021:

- Phase behaviour measurement of ternary systems contain CO_2 and two components, each with a different functional group
- Thermodynamic modelling of ternary systems contain CO_2 and two components with state of the art / models in process simulators

Project available at Mastes and PhD level

- Masters requirements: BEng or equivalent with 65 % average
- PhD requirements: MEng or equivalent with 65 % average

Funding available depending on student profile

Application: Please send your CV including detailed academic transcript to Prof. Schwarz.