

## Master Thesis (experimental / theoretical)

### Experimental investigation and model adaptation for dynamic phase separation in microemulsion systems

#### Research background:

In the research cluster Transregio 63 – InPROMT we are investigating homogeneously catalysed processes in liquid multiphase systems. In particular we are looking at the reductive amination of long chained aldehydes in microemulsion systems and are implementing the process in a mini-plant. The Idea behind using a microemulsion system is to use the advantages of a very efficient homogeneous catalysis and combining them with a simple phase separation step for a reliable recovery of the catalyst. The advantage of a microemulsion system is that the phase state (2 or 3 phase) is temperature dependant and can be switched by changing the Temperature.

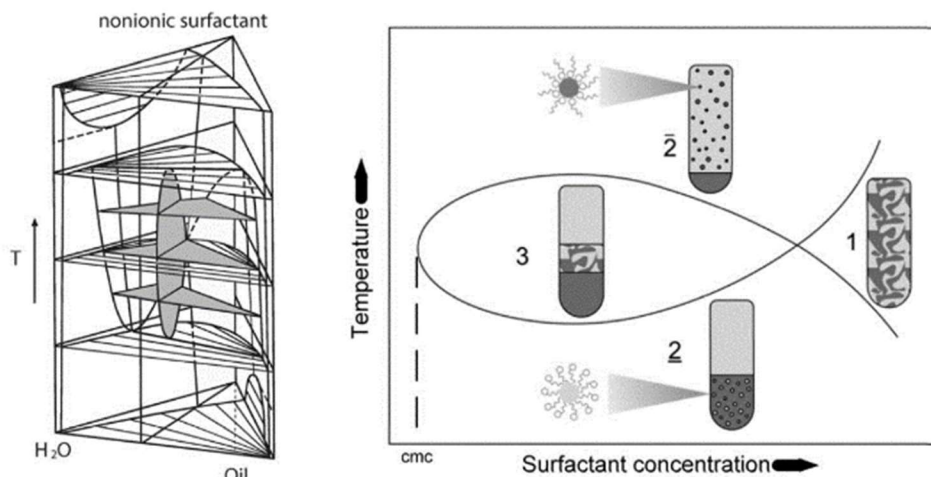


Abb1: Temperatur- und Konzentrationsabhängige Ausbildung von Phasentrennzuständen einer Mikroemulsion bestehend aus Öl/Wasser/Tensid. Abgeändertes Material nach [1].

#### Task:

For the online process optimisation in our mini-plant a complete mathematical model of all process steps is needed. The focus of this work will lie on the development and adaptation of a dynamic phase separation model.

The following aspects will be investigated:

- Experiments for phase separation with real reaction mixtures for the reductive amination in an existing lab setup
- Adaptation of an existing phase separation model for the hydroformulation to fit the new reaction system
- Parameter estimation with experimental data
- Model validation in a mini-plant trial

The thesis can be written in either German or English

**Motivation:**

After finishing this thesis, you will have a deeper understanding of model development, empirical adaptation and parameter estimation; understand reductive amination reactions and how microemulsion systems work; have experience in solving industry related tasks; experience what it means to work with a real mini-plant, its Process Control System (PCS), OPC and OPC UA data exchange protocols.

**Skills and Knowledge:**

You can successfully complete this thesis if you have experience in the lab; have an understanding of thermodynamics, basic chemistry/reaction engineering, model development and numerical methods; and have basic programming skills, preferably python (or matlab).

**Contact:**

**Karsten Duch**

**FG Dynamik und Betrieb technischer Anlagen**

**Tel.: 030 314 70424**

**Email: [karsten.duch@tu-berlin.de](mailto:karsten.duch@tu-berlin.de)**

[1]: Stubenrauch, C. Microemulsions: Background, New Concepts, Applications, Perspectives; Stubenrauch, C., Ed.; John Wiley & Sons, Ltd.: Chichester, U.K., 2009.