

## **Master Thesis**

## **CFD-Simulation of a phase transfer reaction**

Hydrogen storage in a fossil-free world requires liquid derivatives such as methanol and ammonia. However, the synthesis of these molecules takes place in a gaseous environment at high temperature, whereas the advantage of the molecules in a hydrogen economy is in the liquid phase. The condensation of these molecules in simple geometries using cooling water reduces the overall process efficiency due to the loss of high temperature heat. Therefore, new designs for condensation devices are being investigated. In the design, multiphysics simulations play a crucial role to account for all important phenomena such as fluid flow, mass and heat transport, and phase transfer.

This master thesis is embedded in a research project together with Siemens, which focuses on the establishment of new structures for efficient heat management using 3D printed structures. Heat management in Power-to-X technologies plays an important role on the way to competitiveness with traditional synthesis routes. The aim of this thesis is the implementation of a phase transfer model for the methanol synthesis in the software StarCCM+. CFD simulation solving fluid flow and heat transfer shall be combined with thermodynamic equation of state to consider vapor-liquid equilibria.

**Topics:** CFD-simulation, Methanol synthesis, Equation of states, Process design, Heat exchange, Multiphase flows



## **Qualifications:**

- Experience in process and CFD-simulation (ideally either in COMSOL Multiphysics or StarCCM+)
- Ability to work independently as well as in a group environment
- Personal initiative and creativity in new fields of research
- Proficiency in fundamentals of fluid dynamics and thermodynamics
- Critical thinking and interpretation, as well as presentation of research results



Fürth, Dr.-Mack-Str. 81, Technikum 2 5 minutes from U1 station *Stadtgrenze* 



Leon Kick, M.Sc.

leon.lk.kick@fau.de

**+49 (9131) 85-65117** 



From January 2025



Chair of Power-to-X Technologies Correspondence **Prof. Bastian JM Etzold** FAU / Power-to-X Technologies Dr.-Mack-Str. 81, 90762 Fürth