

Master's thesis

## Particle-resolved CFD simulation for methanation in fixed-bed reactor

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### Content:

Heterogeneous catalytic methanation is an essential process in Power-to-Gas technology. A critical challenge of this process is maintaining the temperature below the catalyst limitation to prevent sintering due to high reaction temperatures (hotspot temperature). Particle-resolved CFD simulation can accurately model the condition of all catalyst particles within a fixed bed, providing detailed insights into the internal heat transfer processes. This method allows for precise identification of hotspots within the fixed-bed methanation process.

For this research, the primary purpose is using the particle-resolved CFD to simulate the methanation reaction within a fixed bed, identify the hotspots, and analyze the temperature and the distribution of various gaseous components. Subsequently, particle-resolved CFD simulation will be compared with simpler effective homogeneous simulation to identify ways to improve the latter. The goal is to ensure that the effective homogeneous CFD simulation closely mirrors the results from the particle-resolved CFD simulation, particularly in terms of hotspot prediction and overall temperature distribution trends.

### Tasks:

- Literature research: catalytic methanation, kinetic models, and relevant simulation.
- CFD simulation in ANSYS Fluent with methanation kinetic models.
- Comparison of particle-resolved CFD simulation and effective homogeneous CFD simulation for methanation in fixed-bed reactor
- Written documentation of the thesis.

### Your profile:

- Basic knowledge of CFD-Simulation (favorable but not mandatory)
- Working independently
- Teamwork with the supervisor

### Start: from now

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