



# Master's Thesis

(Theoretical)

## Waste-to-X: Systematic Comparison and Modeling of Reaction Mechanisms in the Gasification of Residues

### Description:

In view of the climate-driven transition in resources and energy, as well as the high dependency on imports of fossil raw materials, the development of new resources such as biogenic residues or plastic waste is of utmost importance. Closing the carbon cycle also represents a crucial aspect in making the chemical industry more sustainable. One promising approach is entrained flow gasification, which enables the conversion of residual materials or biomass into high-quality synthesis gas ( $H_2$  &  $CO$ ). This gas can then be used, for instance, in IGCC power plants for electricity generation or in catalytic syntheses to produce basic chemicals like methanol or Fischer-Tropsch (FT) products.

The complete conversion of fuels in entrained flow gasifiers largely depends on the heterogeneous reaction between the solid material and the gasifying agent. The complex pathway of this reaction step remains unresolved, with various reaction mechanisms proposed in the literature. The quality of models used to describe gasification processes is therefore highly dependent on the selected reaction mechanism for representing the surface reactions during gasification.

The aim of this work is to compare different reaction mechanisms and assess the modeling accuracy against experimental data. As a first step, a comprehensive and systematic literature review of available reaction mechanisms and their applications will be conducted. Furthermore, models for different mechanisms will be developed and tested for their ability to represent experimentally determined reaction kinetics. The ambition of this work is to identify suitable mechanisms for modeling gasification reactions and kinetics. The results will be compared with existing literature and documented in writing.

### Requirements:

- Independent way of working
- Reliability and personal responsibility
- Programming skills desirable

### Work Packages:

- Familiarization with reaction kinetics, particularly of entrained flow gasification
- Systematic investigation of gasification reaction mechanisms
- Development of models for kinetic modeling based on various reaction mechanisms
- Documentation of work and regular meetings with the supervisor

**Start:** 01.06.2025

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