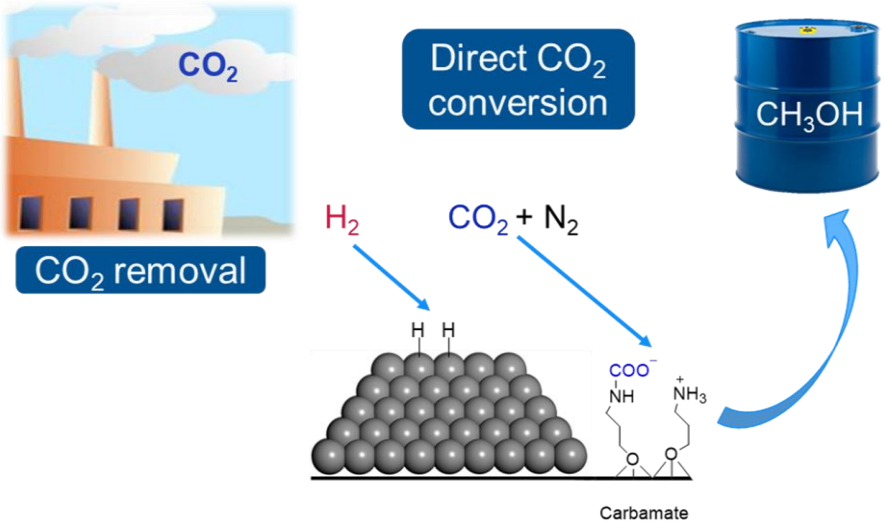
Institute for Chemical Technology and Polymer Chemistry
Department Chemical Technology
Prof. Dr. Olaf Deutschmann

Master Thesis

Modeling and Simulation of CO_2 Capture and Methanol Synthesis

Motivation/Background

CO_2 capture and utilization can be combined in a one-step process to novel pathways for chemical synthesis, which present an alternative to the frequently criticized CO_2 sequestration. Particularly, CO_2 is captured on a dual functional material and subsequently converted with renewable H_2 to MeOH via selective dehydrogenation of captured CO_2. This capture/conversion concept allows to remove CO_2 from flue gas streams of localized sources (e.g. power plants, NH_3 synthesis, cement production) by sorption processes without requiring an energy intensive desorption step for CO_2 and to valorise it to methanol.
The mechanism of the hydrogenation of CO_2 to methanol over the proposed bifunctional materials relies on the combination of sorption processes and catalytic processes. Achieving high yield and selectivity require a thorough understanding of the mechanism.



Description of Work

The work plan includes the development of a kinetic model consisted of elementary-step reactions on both types of active sites. Numerical simulations using appropriate reactor models will enable the validation of the kinetic model via comparison with experimental data (experiments not part of this thesis). The model will be used to simulate the performance under CO_2 capture as well as under the 2-step methanol production conditions (transient simulations).

Contact/Supervision

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