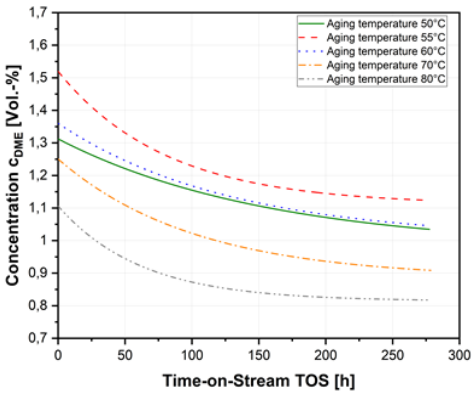
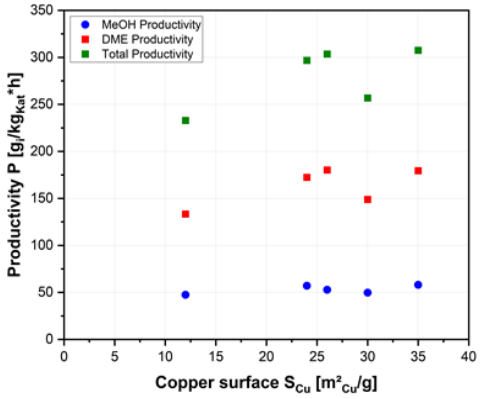
Experimental and Simulation Studies of Methanol and DME Synthesis from CO_2-rich Syngas on Cu/ZnO/ZrO_2 Catalysts

M. Herfet[1], B. Campos[1], K. Herrera Delgado[1], M. Kind[2], S. Polierer[1], J. Sauer[1], L. Warmuth[1], S. Wild[1], T. Zevaco[1] and S. Pitter[1]
Karlsruhe Institute of Technology - [1] Institute of Catalysis Research and Technology - [2] Institute of Thermal Process Engineering

Abstract

Methanol and dimethyl ether (DME) are important “Power-to-X (PtX)” products used as intermediates in the production of CO_2-neutral fuels and base chemicals. New applications in the chemical industry and heavy-duty transportation have led to numerous research activities regarding the synthesis of these two chemicals, in order to maximize the production efficiency. Both methanol and DME can be directly synthesized from H_2/CO_x streams derived from a variety of feedstocks. However, the CO/CO_2 ratio has a particular impact on the process conditions, which might cause in reduced carbon utilization and loss of catalytic activity. Understanding the main path of activity degradation (e.g., figure 1) would also allow for precise optimization of process parameters and further improvement of the process efficiency (e.g., figure 2) as well as economic feasibility under variable conditions.





The aim of our research is to improve the catalyst stability and its activity at variable $CO/CO_2/H_2$ feed compositions. A quantitative description of the catalyst behavior by kinetic and surface activity models is also studied by using multiscale modeling.
For the experiments, different in-house prepared Cu/ZnO/ZrO_2 (CZZ) catalysts for methanol synthesis and a commercial zeolite (H-FER-20) as dehydration catalyst were used. The catalyst screenings were performed in a miniplant with six parallel fixed bed reactors at variable reaction conditions (i.e., temperature, feed compositions, pressure and weight-hourly-space-velocities). To get knowledge of the catalyst stability we performed experiments over 300 h time on stream (TOS). Hereby, we focus on the determination of product selectivity and catalysts activity in CO_2-enriched syngas feeds and the distinct role of water as byproduct potentially affecting the intermediates on the catalyst surface and therefore the reaction kinetics, as well as the state and morphology of the catalytic surface itself.