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Kinetic Evaluation of Light Olefin Synthesis from Syngas using Tandem Catalysis.

Keywords: syngas to olefins, metal oxides, zeolites, kinetic evaluation, kinetic modelling

Aim

Experimental kinetic evaluation of an oxide-zeolite catalyst for direct synthesis gas $(CO_x + H_2)$ conversion into light olefins. Addressing the kinetics of the syngas conversion through the development of a kinetic model, providing a foundation for process optimization and further scale-up studies.

Justification

The production of light olefins, essential building blocks for numerous chemicals, plays a crucial role in the modern chemical industry. Traditionally reliant on fossil crude oil as the primary source for chemicals and fuels, our global society is now at a turning point. Oil production is peaking with highly volatile prices. In this context, exploring alternative raw materials such as petcoke, coal, natural gas, biomass, and solid waste becomes increasingly important. However, the only feasible pathway to valorize some of these alternative resources at a commercial scale is via the initial conversion into syngas. This syngas is then converted into other chemicals such as methanol, and long (saturated) hydrocarbons (via Fisher-Tropsch synthesis), yet excluding light olefins which are of particular interest to TotalEnergies as the partner in this project.

Although Fisher-Tropsch synthesis with Co- and Fe-based catalysts was considered promising for the Syngas-to-Olefin (STO) reaction, their selectivity for C_2-C_4 hydrocarbons is relatively limited, not exceeding 58%, in accordance with the Anderson-Schulz-Flory (ASF) distribution.



To enhance the lower olefin yield, recently bifunctional oxide-zeolite (OX-ZEO) catalysts with ZnCr oxide and SAPO-34 zeolite have emerged, exhibiting a remarkable selectivity amounting to 80% for C_2 – C_4 olefins, well above the ASF limit. A promising one-step approach to convert syngas into light olefins involves the combination of methanol synthesis over metal oxides, which do not promote hydrocarbon chain growth, with a small-pore zeolite that selectively converts the formed methanol into light olefins (MTO). Despite the remarkable performance of

ZnCr/SAPO-34 bifunctional catalysts, practical application remains a challenge due to the harmful Cr component and migration of Zn species, which deteriorates light olefin productivity over time. To overcome these issues, a high-performance, Cr-free OX-ZEO catalyst with remarkable stability, even at high CO_x conversion levels, has been developed.

This thesis aims to develop a kinetic model for this reaction, utilizing high-throughput experimentation to accelerate data acquisition. By refining the kinetic understanding, this study will support process optimization and scale-up efforts.

This master thesis project gains unique significance through its collaboration with TotalEnergies. The strategic interest of TotalEnergies underscores the project's practical relevance and potential impact on the chemical industry.





Program

- Literature review focused on the reaction mechanism and kinetic model development.
- Utilization of a high-throughput kinetic screening setup with 4 parallel reactors to analyze the performance of the OX-ZEO catalyst and acquire reliable kinetic data.
- Development of a kinetic model with the aim to optimize the process variables, ultimately supporting the industrial application of OX-ZEO catalysts for light olefin.

