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Coach	Supervisor(s)	Funding
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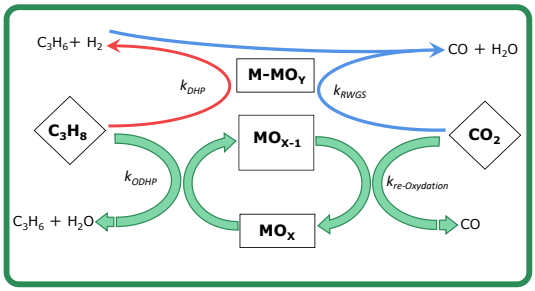
"Kinetic modelling analysis of Vanadia-Based(V/CHA) Catalysts on CO_2-Assisted Oxidative Propane Dehydrogenation"

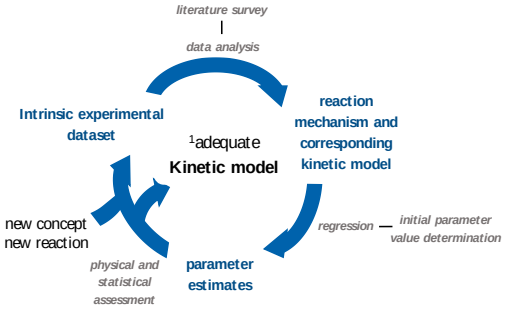
Aim

The aim of this project is to conduct a comprehensive theoretical kinetic investigation of CO_2-Assisted Oxidative Propane Dehydrogenation (CO_2-ODHP), focusing on the production of propylene using V/CHA Vanadia-Based Catalysts.

Justification

The increasing global demand for propylene, a key component in the chemical industry, is at odds with the environmental impact of traditional production methods, such as steam cracking (SC) and Fluid Catalytic Cracking (FCC). These methods, particularly SC, face a 'propylene gap' due to a shift towards ethane-rich shale gas, particularly in the USA, leading to lower propylene yields. Additionally, the high CO_2 emissions associated with these methods conflict with the growing demand for sustainable industrial practices and the escalating costs of carbon emissions. In response to these challenges, the proposed master thesis project focuses on the Oxidative Dehydrogenation of Propane (ODHP) as a transformative process for Propane Dehydrogenation (PDH). ODHP is renown for its low energy requirements, elimination of catalyst regeneration, and absence of thermodynamic constraints. By potentially converting existing PDH plants, it offers a cost-effective solution. Moreover, utilizing CO_2 as a mild oxidant in ODHP not only favors olefin production but also contributes to CO_2 consumption and CO production, aligning with the aim of reducing CO_2 emissions and utilizing CO as a sustainable chemical feedstock.





V/CHA Vanadia-Based Catalysts are promising for ODHP-CO2 due to their high activity at temperatures below 600°C and high propylene selectivity (>80%). However, in order to offer a viable, scalable, and more eco-friendly alternative a detailed kinetic analysis is mandatory. Current literature on ODHP kinetic modelling is limited, and existing models exhibit several shortcomings, including inadequate description of the products distribution, undefined kinetic steps in the reaction mechanism and lack of statistical and physico-chemical analysis in model development. This work aims to address these gaps through a combined theoretical and experimental kinetic analysis.

Program

- Conduct a focused survey of kinetic studies on CO_2-ODHP, identifying research gaps.
- Experimental verification of the CO_2-ODHP using V/CHA Catalysts
- Formulate potential reaction mechanisms for CO_2-ODHP, highlighting the role of V/CHA catalysts.
- Develop and construction of kinetic models using elementary steps to describe CO_2-ODHP experimental observations.

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