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Coach	**Supervisor(s)**	**Funding**
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Effect of zeolite topology in methanol-to-olefins conversion

Aim

Understanding the effect of zeolite topology on the reaction mechanism in methanol-to-olefins

Justification

Due to the fluctuation of oil prices and an increased environmental awareness, research on sustainable alternatives to crude oil as a feedstock has become increasingly important. Among the commercially relevant olefins, the global demand of propylene has increased most significantly. The alternative process of interest is the developed methanol-to-olefins process over a heterogeneous catalyst. Porous solid zeolite catalyst with high porosity such as H-ZSM-5 or H-SAPO-34 convert methanol into light olefins and hydrocarbons with a wide range of applications as depicted in Figure 1 [1].

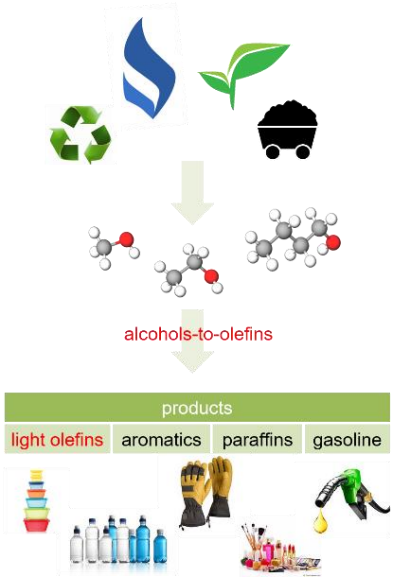

Figure 1: Schematic representation of the methanol-to-olefins process with corresponding applications

To improve activity and increase the propylene yield, the elucidation of the relation between zeolite topology (i.e., structure) and the reaction mechanism is required to improve activity and increase the propylene yield [2]. Currently, the dual cycle mechanism involving aromatics and alkenes is getting widely accepted [1]. The extent to which both cycles contribute to the overall product formation, which depends on the zeolite topology and operating conditions, is still to be resolved. The effect of zeolite topology on the catalyst activity and selectivity will be investigated for different zeolites through intrinsic kinetic data acquisition and demonstrated with a kinetic model.

Program

Prior to the start of this thesis, intrinsic kinetic data will have been gathered for methanol-to-olefins on H-ZSM-5 (Si/Al=40,25 and 140) [3, 4]. In the present thesis, additional kinetic data will be acquired for zeolites with different structure (H-ZSM-5, H-beta and H-SAPO-34) to be benchmarked against methanol conversion over the catalyst H-ZSM-5 (with Si/Al=40). The performance of methanol over different zeolites will consequently be tested on the high-throughput mechanistic investigation set-up to give insights into the relative importance of the catalytic cycles. The global trends of the mechanism will also be described by a kinetic model.

[1] U. Olsbye, et al., Angewandte Chemie-International Edition, 51 (**2012**) 5810-5831.
[2] U. Olsbye, et al., Catalysis Today, 106 (**2005**) 108-111.
[3] B. Pessanha., *A steady State Study: Effect of Zeolite and Operating Conditions on Methanol-to-Olefins* (Master's thesis), Instituto Superior Técnico, Lisbon, Portugal (2019)
[4] T. Lei., *On reaching steady-state in methanol-to-olefins experimentation: effect of hydrocarbon pool species* (Master's thesis), Ghent University, Ghent, Belgium (2020)

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