LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	**Supervisor(s)**	**Funding**
dr. ir. Pieter Janssens	prof. dr. ir. Joris Thybaut dr. ir. Jeroen Poissonnier	

Elementary-kinetics driven catalyst design methodology applied to the Fischer-Tropsch synthesis of light olefins at high-temperature conditions

Aim

Development of a kinetics-driven catalyst design methodology applied to the Fischer-Tropsch synthesis (FTS) of light-olefins at high-temperature Fischer-Tropsch (HTFT) conditions. The methodology establishes relationships between catalyst-invariant model parameters, i.e. catalyst descriptors, and structural properties of the catalytic material using the concept of virtual catalyst screening. Subsequent extraction of the optimal catalyst descriptor values then yields **next-generation FTS catalysts**.

Justification

Ill-defined relationships between model parameters and structural properties limit the rational design of next-generation catalysts for many reactions, including FTS. While Density Functional Theory has emerged as a potential solution, several limitations remain such as for extended reaction networks. Data science has proven to be occasionally successful as well, however, it requires large datasets and does not bring the desired mechanistic insight. The development of a kinetics-driven catalyst design methodology will allow mitigating these issues by establishing descriptor-property relationships. A proof of concept of such a methodology has recently been reported by Pirro et al. [1] which relied on a Single-Event MicroKinetic (SEMK) model embedded in an iterative virtual catalyst screening cycle, using well-chosen data mining and statistical tools, and exhibits a broad applicability based on a (very) limited experimental input.

This virtual catalyst screening cycle yields descriptor-property relationships which allow to translate descriptor values into measurable and tunable features of the catalyst. The concept can be transformed into a catalyst-design methodology if the optimal descriptor values for a (set of) performance-indicator(s) (e.g. conversion or selectivity) for an application of interest can be obtained. Light olefins such as ethylene and propylene are important platform chemicals and in this thesis proposal, the aforementioned design strategy will be applied to the iron-catalyzed FTS of these products at HTFT conditions.

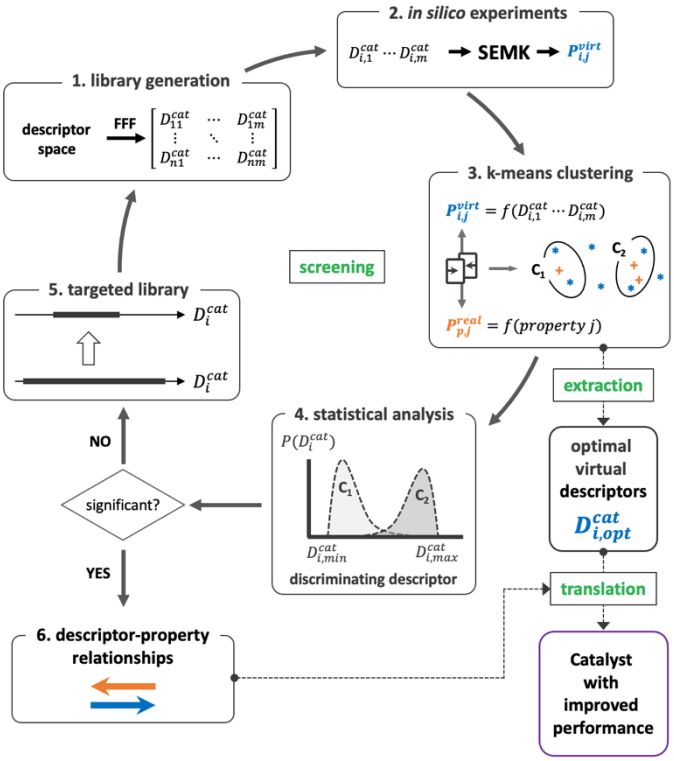

Figure 1 Envisioned kinetics-driven catalyst design methodology

Program

- Literature survey on (micro)kinetic catalyst-design methodologies and FTS of light olefins.
- Development of the catalyst-design methodology:
  - Single-workflow virtual catalyst **screening** cycle based on a SEMK model for FTS.
  - Automated **extraction** of optimal descriptor values, applied to the HTFT synthesis of light olefins, starting from on a very small dataset available in the literature.
- **Translation** the optimal descriptor values into a FTS catalyst with improved performance.

[1] L. Pirro et al. "Descriptor-property relationships in heterogeneous catalysis: Exploiting synergies between statistics and fundamental kinetic modelling," *Catal. Sci. Technol.*, vol. 9, no. 12, pp. 3109–3125, 2019.