LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125 9052 Gent, Belgium

Coach	Supervisor(s)	Funding
Pieter Janssens César Pernalete	prof. Joris W. Thybaut	IOF and VLAIO

Controlling Industrial-Scale Catalyst Deactivation in Hydroprocessing

Aim

Develop, implement and validate industrially relevant structure–activity relationships (SARs) for catalyst deactivation in hydroprocessing via accelerated deactivation experiments and/or microkinetic modeling.

Justification

The oil refining sector faces growing challenges as refineries must process increasingly complex feedstocks. Light, clean crudes are becoming scarce, pushing the industry toward heavy, unconventional oils such as sand and shale oil. To meet product specifications, refineries rely heavily on hydroprocessing (HP) units, e.g., hydrotreaters and hydrocrackers, that catalytically upgrade and convert intermediate streams using hydrogen. These units influence nearly all fuels and chemicals produced, see Figure 1. Process modelling plays a critical role in refinery decision-making processes. Current modelling tools perform well for limited feed variability but struggle with complex feedstocks and tighter quality requirements. To address this, we have developed a Single-Event Microkinetic (SEMK) software that allows reliable management of such complex feedstock mixtures. This software has proven very effective for modelling a large industrial hydrocracker [1].

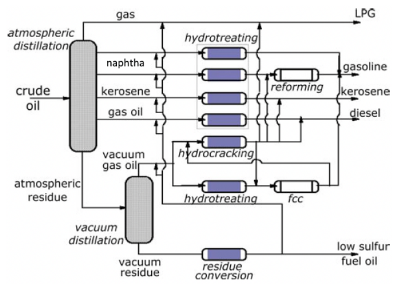

Figure 1: conceptual refinery lay-out

A key capability requested by industry is accurate catalyst deactivation modelling. Catalyst lifetimes range from months to years (Figure 2), and replacing them requires a plant shutdown, making cycle-length prediction critical for planning and profitability. However, modelling deactivation is difficult due to the many interacting mechanisms and the vastly different timescales on which the phenomena take place. Our approach will therefore rely on **accelerated deactivation experiments** on industrial catalysts provided by our industry partners. This will allow us to develop **structure–activity relationships (SARs)** that will be **incorporated into the SEMK software** for validation and to deepen fundamental insights into HP deactivation (i.e., mechanism elucidation).

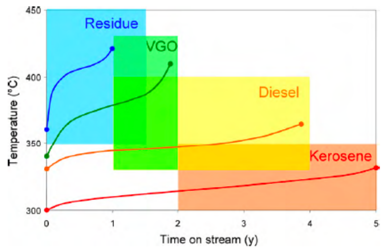

Figure 2: catalyst operating cycles in HP

Program

The focus of the thesis will be tailored to the preference of the student. More specifically, in the general program shown below, the student is free to choose between **Option 1** and **Option 2**, or a combination of both.

- Literature study: state-of-the-art on catalyst deactivation experimentation and/or modeling.
- **Option 1: SARs development [experimental focus]**
  - accelerated deactivation on industrial-grade hydrotreating and hydrocracking catalysts
  - analysis of the physicochemical properties of fresh and spent catalysts
- **Option 2: SARs implementation and validation [modeling focus]**
  - implementation of deactivation pathways and selected catalyst properties into a SEMK model
  - in-depth comparison of the improved model performance on industrial hydrocracker data
- Optional: communicate on the obtained results during interactions with our industrial partners

references

[1] C. G. Pernalete.,S. Zahedi Abghari, P. Janssens, K. M. Van Geem, J. W. Thybaut. Ind. Eng. Chem. Res. (2024). Vol. 63. pp 21841-21859

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