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Implementation of desulfurization and denitrogenation kinetics in hydrotreating and –cracking reactor modeling

Aim

The aim of this thesis is to develop a kinetic model inspired on the Single Event MicroKinetics methodology to simulate hydrodesulphurization (HDS) and hydrodenitrogenation (HDN) reactions in the context of vacuum gas oil hydrotreatment (HDT).

Justification

HDT processes are core units in modern oil processing plants. In refineries, upgrading steps and even in state-of-the-art chemical plants configurations, these processes are key for the manufacturing of a great variety of products. Fuels, synthetic crude oil and lube oils are produced using HDT units as part of the refining scheme.

The trend in the oil industry is to process increasingly heavy feeds. Along with that, the heteroatom content is typically higher, sulfur and nitrogen species being the most common ones. The purpose of the HDT processes is to remove these heteroatoms, since they cause catalyst poisoning downstream and contribute to the generation of air pollution. When sulfur and nitrogen levels in the end products exceed the regulation limits, a large amount of SOx and NOx would be produced in the combustion step of the fuels.

With the purpose of having a software tool that allows to represent the HDT process for vacuum gas oil (VGO), it is necessary to develop a kinetic model for the HDS and HDN reactions. The objective is to have a fundamental insight in these mechanisms using the Single Event MicroKinetics methodology. These reactions will be included in an existing framework that models other reactions occurring during the refining of VGO. The developed kinetics will be validated by comparison against experimental data available at LCT.

Program

1. Literature review about HDS, HDN, HDT kinetic modelling.
2. Definition of the single event kinetic model to be implemented.
3. Implementation of the model as part of the general framework of reactions for the treatment of VGO.
4. Validation of the developed model using available data at LCT.
5. Case study using the developed model.