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An interpretable machine learning approach coupled with microkinetic modeling to enhance light olefin production in Fischer Tropsch Synthesis

Aim

Investigation of the possibility of using “black-box” machine learning models like Deep Neural Networks (DNN) for the identification of the optimal operating conditions for Fischer-Tropsch synthesis (FTS) for enhanced light olefin production over iron based catalysts. Different statistical techniques will be used to extract insights from sophisticated machine learning models to construct an **model that can be fundamentally interpreted**, rather than the traditional black-box models.

Justification

At present, kinetics-driven models such as Single Event Micro-Kinetic model (SEMK) are extensively used to explain the detailed multiscale phenomena of various catalytic reactions, such as the FTS which plays a crucial role in attaining circular economy. These micro-kinetic models are used to analyse the influence of different catalyst properties on their activity and selectivity towards different desired products. They allow calculating the conversion and selectivity obtained at different operating conditions, and with different catalysts. However, the reverse process, i.e. the identification of the optimal operating conditions required to maximize the desired product yields using the microkinetic models requires human intervention.

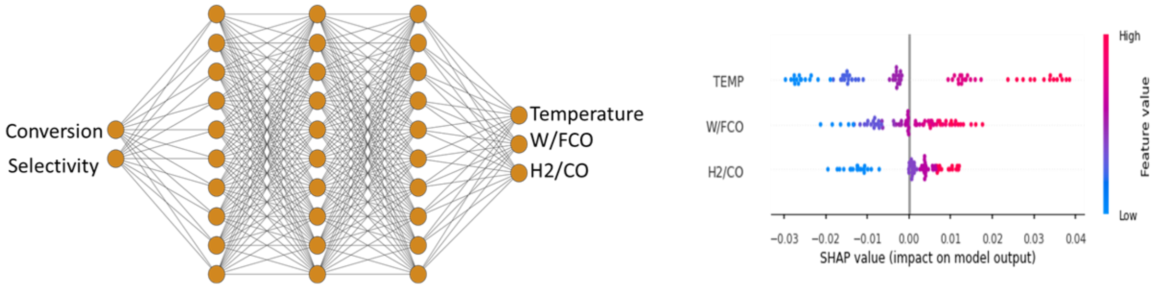

*Figure **Error! No text of specified style in document.**-1: a) Deep Neural Network prediction b) Feature importance for FTS process.*

Recently, machine learning (ML) methods like DNN have gained popularity and have performed as powerful predictive tools in various areas of academic and industrious activities. However, their application in catalysis is under-developed due to their black box character. Black box models like DNN gives the functional relationships between system inputs and system outputs, and does not explain the physico-chemical significance of process parameters. In the current work, we investigate the possibility of using DNN to further assist the capabilities of microkinetic models to automatically identify optimum operating conditions (Fig.1.a). The DNN will be trained using the outlet flow rates obtained from experimental data and SEMK model simulations, to predict the optimum conditions. To interpret the black-box DNN model statistical tools will be applied to answer the following questions:

- What features in the data are identified as most important by the model?
- How did each feature in the data affect the corresponding prediction?
- How does each feature affect the general model prediction capabilities?

The solutions to these questions will assist the development of an interpretable machine learning (Fig.1.b) and the SEMK model. This will be the next step towards a true circular economy by maximizing the light olefin production from the FTS of syngas generated via gasification of plastics, as envisaged in the PSYCHE project.

Program

- ➢ Literature survey on (micro) kinetic models, machine learning models and coupling thereof.
- ➢ Development and extension of existing Python scripts for Machine learning.
- ➢ Identification of optimal FTS operating conditions and cross verification with the SEMK model.