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Automated construction of kinetic models from catalytic experimental data

Aim

Automate the construction of kinetic models by developing an algorithm able to translate experimental kinetic information into reaction rate rules.

Justification

The development of a whole new generation of catalysts suitable for sustainable processes is crucial. Kinetic modelling has frequently been postulated as the ideal tool for catalyst design. Indeed, the use of fundamental relationships, particularly when based on detailed kinetic models, enables the identification of the optimal catalyst structures, set of operating conditions, and reactor configuration [1]. However, constructing a kinetic model requires expertise and can become a time-consuming task, **liming the use of kinetic modelling for catalyst design** up to now. Furthermore, due to the increased availability of open data [2], even faster generation of kinetic models will be required.
In this work, the goal is to **automate the model construction** based on the extracted information.

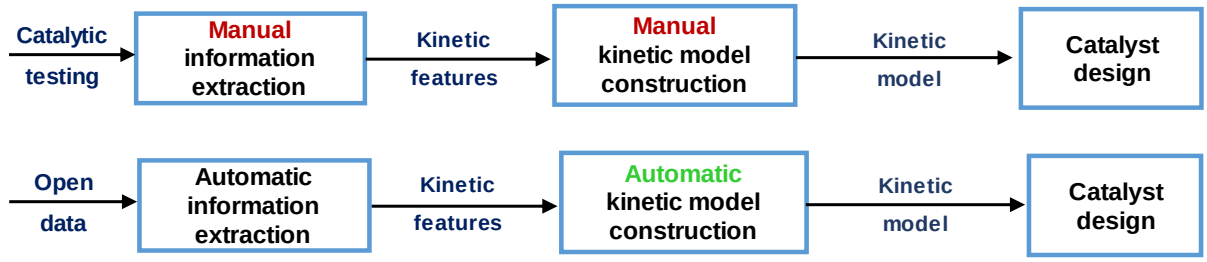

Figure 1: Simplified flowchart for kinetic modelling. Top: typical approach (bottlenecks in red). Bottom: automated approach under development at LCT (innovations foreseen in the master thesis in green).

Program

Develop a software with the capability of constructing kinetic models from kinetic information retrieved in experimental data. In practice, this means that the kinetic information consisting of the main patterns in data will need to be translated into chemical phenomena which will ultimately lead to a rate equation. The starting point will be the most simple catalytic type of rate equations: the so-called Langmuir-Hinshelwood-Hougen-Watson models. For these cases, the visual identification of the rate equations based on well-selected plots has been originally proposed [3] and can then be used to generate chemical rules that translate kinetic information into rate equations. The developed algorithm will expand and complete a recently developed Python software to extract automatically kinetic information from experimental (open) data [4].

[1] K. Van der Borght, K. Toch, V. Galvita, J. Thybaut and G. Marin, *Catalysts*, 2015, **5**, 1948.
[2] https://www.openaire.eu/
[3] K. H. Yang, O. A. Hougen, *Chemical Engineering Process,* 1950, **46**, 146.
[4] S. Siradze, Automated kinetic feature extraction from Open Access data, MSc thesis, 2019, Ghent University.

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