Advantages of AI-based regressions for the kinetic modelling of industrial catalysts

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In industrial practice, commercial catalysts are the best choice to build effective chemical plants. Unfortunately, due to their complex compositions and properties, the definition of the reaction mechanism and intermediates is often difficult. Therefore, the development of robust kinetic models is challenging, which limits the reliability of reactor design practices. This raises the question of whether AI-based regressions could give reliable regressions of kinetics without requiring detailed reaction mechanisms.

This research question was addressed by performing kinetic experiments on a commercial CO_2 methanation Ni/ZrO_2 catalyst in an isothermal, fixed bed reactor. Thereby, a dataset of 216 points at various temperature (220-300 °C), partial pressure (0.8 – 3 bar) and gas hourly space velocity (50,000 – 700,000 h^{-1}) was obtained. The results from machine learning-based regressions were compared with Langmuir-Hinshelwood-Hougen-Watson (LHHW) models from literature. AI-based regressions were trained on this dataset, and their goodness of fit was assessed with root mean squared error. Four models: power law, Gaussian Process Regression (GPR), 1-layer neural network (ANN) and a LHHW model were selected.

In Figure 1, the power law (a) displays an inaccurate fitting due to its scarce capability in describing the complex interplay of adsorption sites on a catalyst for CO_2 methanation. By comparison, the AI-based models (b, c) show excellent fits of the experimental results. The fit of the not shown LHHW model is good but was only obtained after extensive research to determine which mechanistic model best described the catalyst.

The sensitivity of fit appropriateness was then measured by modifying the size of the dataset. The AI-based models were more robust than the LHHW model with reduced amounts and types of data used for their regression. The models were later used in a reactor design phase, to assess their influence on the simulation of a full-scale reactor. Using the experimental dataset, both approaches suitably described the performance of a CO_2 methanation reactor.

This work shows the potential of using AI-based regressions for kinetic modelling of industrial catalysts, especially those lacking mechanistic information. This approach shows potential in accelerating the reactor design phase for many catalytic processes, where the mechanistic analysis is challenging.

Keywords: Kinetic modelling, CO_2 methanation, machine learning, industrial chemistry

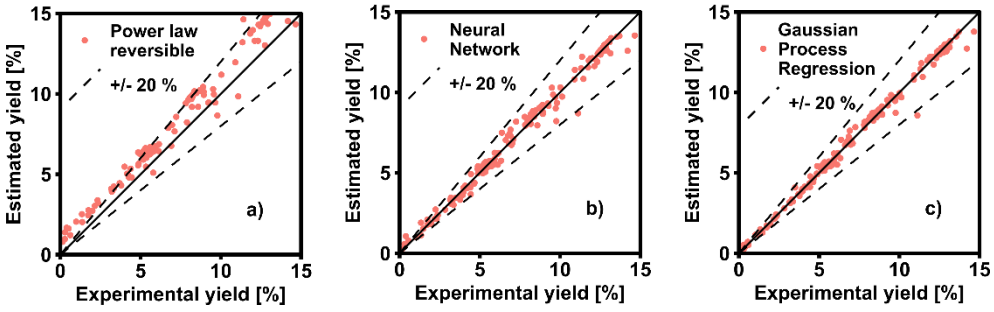

Figure 1. Parity plots of the power law (a), 1-layer neural network (b) and GPR (c), under 15 % methane yield.