ANN-based surrogate modelling for short- and long-term performance optimization of CO_x methanation reactors

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This study focuses on the application of artificial neural networks (ANNs) to the dynamic surrogate modelling of chemical reactors. Fixed-bed CO_2 methanation is used as case study, due to the dynamic and variable nature of green hydrogen input. A mechanistic model was validated against experiments and used for the generation of a training dataset for two types of ANN-based models:

1. **Feed-forward neural networks (FFNN).** These were applied to model the response of the reactor to a single step change in the inlet flowrate, assuming that the CO_2:H_2 ratio is kept at the stoichiometric ratio of 1:3. A single neural network was designed to model the reactor response at each minute (from 1 to 10) after the step change. Inputs are the initial and final flowrate and outputs are hotspot temperature, conversion and yield in the reactor. This model type showed promising results to describe the short-term response of the reactor, ideal for optimization and control.
2. **Recurrent neural networks (RNN).** These networks are applied to the prediction of time-series data. In this work they were applied to predict the reactor response to a hydrogen flowrate profile over a day. The response was evaluated in terms of hotspot temperature, conversion, and yield.

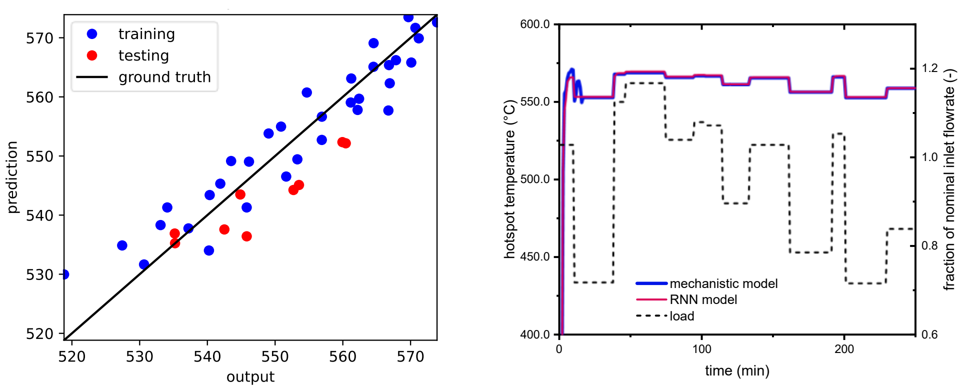

Figure 1: *(a) Parity plot of the FFNN model 1 minute after the step change. (b) Comparison between hotspot temperatures according to mechanistic and RNN models after several changes in inlet flowrates.*

Both models showed promising results in the prediction of the main reactor KPIs. The FFNN is more accurate in the prediction of the immediate response to a single flowrate step change. The RNN responds better to random sequences of inlet flowrate values over a longer period. Therefore, the application of the former in the field of real-time optimization and control will be investigated, while the latter will be dedicated to the prediction of long-term operational profiles for economic evaluation.

Keywords: *reaction engineering, dynamic modelling, artificial neural networks, AI-based modelling*