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Witchcraft with small data

At the Leibniz Institute for Catalysis in Rostock, LIKAT, a doctoral student working with Dr David Linke developed AI models for the Fischer-Tropsch process based on CO_2. The process was originally developed in the 1920s to produce liquid hydrocarbons from carbon monoxide and hydrogen obtained from coal and petroleum. Laboratories around the world are researching ways to use the greenhouse gas carbon dioxide instead of fossil raw materials for Fischer-Tropsch synthesis in the future.

One of the research goals in chemistry is to replace fossil raw materials with climate-friendly and environmentally friendly raw materials. A promising approach is the hydrogenation of carbon dioxide to higher hydrocarbons, known as CO_2 Fischer-Tropsch synthesis (CO_2 FTS). CO_2 and hydrogen (H_2) react catalytically to form synthetic fuel, for example, which contains no sulphur or nitrogen compounds and therefore burns much cleaner than its petroleum-based counterpart. If the hydrogen is also produced from renewable sources, this process is completely CO_2-neutral.

First the data, then the experiment

The number of publications on this reaction is increasing worldwide, and with it the amount of data from experiments. 'Those who analyse this data intelligently can discover hidden connections between catalyst properties and chemical activity,' says LIKAT chemist Dr. David Linke. This is valuable knowledge, but difficult to extract. A case for machine learning and artificial neural networks.

Aleksandr Fedorov, a doctoral student of David Linke, embarked on this pioneering work. The goal of his doctoral thesis was to develop a new catalyst for CO2-FTS and a suitable AI model that could describe the speed of the complex reaction under all conditions. This initially meant spending months collecting and processing data and feeding it into a database. David Linke: 'Even before the first experiment, it is important to know as much as possible. Experiments are expensive and time-consuming."

Highly selective iron catalyst

Both the classic Fischer-Tropsch synthesis and CO_2 FTS often take place in so-called bubble column reactors. The gaseous starting materials, H_2 and CO_2, and later also the carbon monoxide (CO) that forms, work their way through a viscous liquid containing the iron- or cobalt-based catalyst and all intermediate and end products.

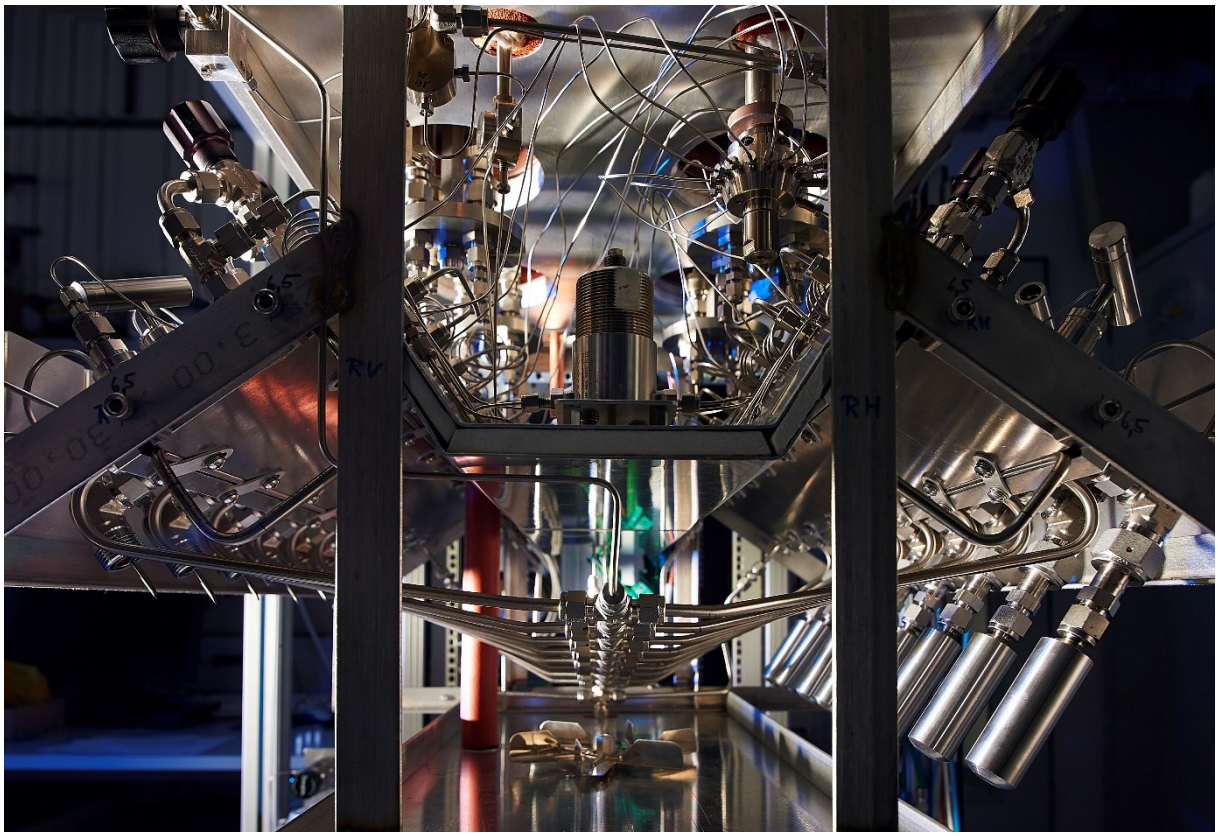

Fig. 1: Effective and attractive: the high-throughput catalytic reactor used by Aleksandr Fedorov. It has 16 parallel reactors – the vessels are clearly visible on the right – and is used to test catalysts for the hydrogenation of CO or CO_2 under pressure. Among other things, the plant enables the conversion of CO into higher hydrocarbons (Fischer-Tropsch synthesis) and the synthesis of methane and methanol from CO or CO_2. Photo: LIKAT

The result of the research work at LIKAT was an iron catalyst with very high productivity and high selectivity that can be activated in the production reactor. High selectivity means that very little unwanted methane is formed in comparison to the desired target products. This was achieved by adding small amounts of potassium, copper and aluminium.

Without much trial and error

To date, chemists have documented their findings on reactions in graphs and tables that illustrate the influence of important parameters such as pressure, temperature and sample composition. Aleksandr Fedorov analysed every single measurement point in around a hundred publications. In doing so, he not only determined the decisive criteria for the effectiveness and selectivity of the reaction. He also uncovered a contradiction: contrary to what is described in the literature, the CO_2 used in the reaction is by no means always converted to CO. This finding opens up a new avenue of research for further catalyst improvement.

Fedorov began training artificial neural networks using data from his catalyst for the kinetic modelling of CO_2 hydrogenation, his AI model. Only a small amount of data was needed because there is always very little laboratory data per measurement series. David Linke: ‘Unlike the usual language AI solutions, the large language models, we work with small data here.’ To

enable the model to calculate plausible reaction sequences, it had to be taught basic physical rules.

The breakthrough came last autumn, as David Linke recalls. ‘Suddenly you get models that behave sensibly! It's a bit like magic.’ Normally, you sit at the computer for days trying to find a suitable model. ‘Now I train the AI model, and even the old laptop calculates everything in 30 minutes.“

Source code as open source

What are the benefits of these AI models? The AI from LIKAT not only reduces laboratory time for further research into CO_2 FTS, but also increases the efficiency of the reaction. Above all, process engineers can now use Aleksandr Fedorov's model to design and build the bubble column reactor much more precisely than before. And anyone can use the model as a matrix to train their own AI for any number of reactions.

David Linke, Aleksandr Fedorov and others have published their findings, including the source code, as open source. As part of the National Research Data Infrastructure (NFDI) founded in 2020, David Linke is convinced that such AI tools will revolutionise the development of chemical processes from the laboratory to the reactor.

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Source code: https://github.com/LIKAT-Rostock/kcnode-paper

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