# Discovery made about Fischer–Tropsch process could help improve fuel production

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A fundamental discovery about the Fischer–Tropsch process, a catalytic reaction used in industry to convert coal, natural gas or biomass to liquid fuels, could someday allow for more efficient fuel production.

Washington State University researchers discovered previously unknown self-sustained oscillations in the Fischer–Tropsch process. They found that unlike many catalytic reactions which have one steady state, this reaction periodically moves back and forth from a high to a low activity state. The discovery, reported in Science, means that these well-controlled oscillatory states might be used in the future to enhance the reaction rate and the yields of desired products.

"Usually, rate oscillations with large variations in temperature are unwanted in chemical industry because of safety concerns," said corresponding author Norbert Kruse, Voiland Distinguished Professor in WSU's Gene and Linda Voiland School of Chemical Engineering and Bioengineering.

"In the present case, oscillations are under control and mechanistically well understood. With such a basis of understanding, both experimentally and theoretically, the approach in research and development can be completely different—you really have a knowledge-based approach, and this will help us enormously."

Although the Fischer–Tropsch process is commonly used for fuel and chemical production, researchers have had little understanding of how the complex catalytic conversion process works. The process uses a catalyst to convert two simple molecules, hydrogen and carbon monoxide, into long chains of molecules—the hydrocarbons that are used widely in daily life.

While a trial-and-error approach has been used in research and development in the fuels and chemical industries for more than a century, researchers will now be able to design catalysts more intentionally and tune the reaction to provoke oscillatory states that could improve the catalytic performance.

The researchers first came upon the oscillations by accident after graduate student Rui Zhang approached Kruse with a problem: he wasn't able to stabilize the temperature in his reaction. As they studied it together, they discovered the surprising oscillations.

"That was pretty funny," Kruse said. "He showed it to me, and I said, 'Rui, congratulations, you have oscillations!' And then we developed this story more and more."

The researchers not only discovered that the reaction develops oscillatory reaction states, but why it does so. That is, as the temperature of the reaction goes up due to its heat production, the reactant gases lose contact with the catalyst surface and their reaction slows down, which reduces the temperature. Once the temperature is sufficiently low, the concentration of the reactant gases on the catalyst surface increases and the reaction picks up speed again. Consequently, the temperature increases to close the cycle.

For the study, the researchers demonstrated the reaction in a lab employing a frequently used cobalt catalyst, conditioned by adding cerium oxide, and then modeled how it worked. Co-author Pierre Gaspard at the Université Libre de Bruxelles developed a reaction scheme and theoretically imposed periodically changing temperatures to replicate the experimental rates and selectivities of the reaction.

"It's so beautiful that we were able to model that theoretically," said corresponding author Yong Wang, Regents Professor in WSU's Voiland School who also co-advised Zhang. "The theoretical and the experimental data nearly coincided."

Kruse has been working on oscillatory reactions for more than 30 years. The discovery of the oscillatory behavior with the Fischer–Tropsch reaction was very surprising because the reaction is mechanistically extremely complicated.

"We have a lot of frustration sometimes in our research because things are not going the way you think they should, but then there are moments that you cannot describe," Kruse said. "It's so rewarding, but 'rewarding' is a weak expression for the excitement of having had this fantastic breakthrough."

**More information:** Rui Zhang et al, The oscillating Fischer-Tropsch reaction, *Science* (2023). DOI: 10.1126/science.adh8463. www.science.org/doi/10.1126/science.adh8463

Provided by Washington State University

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