

PRESS RELEASE

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Digital twin enables increased yield in synthesis processes

Steel production generates large quantities of so-called “furnace gases,” which are rich in hydrogen and carbon oxides. In the [Carbon2Chem® project](#), partners from industry and research are investigating the material utilization of these gases. The Fraunhofer Institute for Solar Energy Systems ISE demonstrated the conversion of purified steel mill exhaust gases into methanol in a mini-plant over a period of more than 5,000 hours. Modeling the process in a digital twin of the plant helped researchers optimize it and significantly increase productivity. The simulation platform developed can now also be used for other applications, such as the production of jet fuels.

Methanol is a basic chemical with high potential as a hydrogen carrier in the energy system of the future. Due to the high greenhouse gas emissions associated with its current production from gas or coal, it must be produced in the future from renewable sources or from carbon- and hydrogen-containing exhaust gases.

Such exhaust gas is available in the steel industry: The smelting of coke and iron ore into steel produces significant amounts of coke oven gas, blast furnace gas, and converter gas. As a result, steelworks are responsible for about six percent of Germany’s CO₂ emissions. The thyssenkrupp Steel Europe steelworks in Duisburg is at the center of the “Carbon2Chem®” research project, in which partners from industry, research, and academia are investigating the material utilization of the aforementioned steelworks gases. In the second project phase, Fraunhofer ISE produced a total of approximately 2,000 liters of crude methanol from purified steelworks gases in a mini-plant.

Digital twin accelerates process optimization

In parallel with this practical work, the institute developed a simulation platform that could be used as a digital twin of the mini-plant for methanol synthesis.

“The basis of the digital twin is knowledge of a kinetic model that describes the underlying reactions with very high accuracy,” explains simulation expert Dr. Florian Nestler from Fraunhofer ISE. “By combining this with a detailed reactor and process model in our simulation program, we can calculate the steady-state and dynamic operating conditions of an entire chemical plant.”

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“On this basis, reliable techno-economic optimizations can be carried out in the next step,” adds Dr. Achim Schaadt, Head of the “Sustainable Synthesis Products” department.

The specific value of a digital twin for a particular plant stems from its adaptation to the plant’s characteristics, such as reactor geometry, the catalyst used, and adjustable operating parameters. Using real measurement data from over 5,000 operating hours of the Miniplant at the steelworks in Duisburg, the digital twin was adapted to the real plant in such a way that it describes the plant’s actual behavior with a high degree of accuracy.

In the next step, the digital twin’s optimization algorithm searched the plant’s operating window for operating parameters that enable particularly high productivity. The algorithm’s suggestions could then be implemented on the plant. Overall, the model-supported optimization was significantly more efficient than a purely experimental search for better operating points.

“We are very satisfied with the practical and simulation results from Carbon2Chem®,” reports project manager Max Hadrich. “Now that our work is complete, we are focusing on collecting comparable data for other products such as dimethyl ether or jet fuels and using our simulation platform for additional digital twins of plants.”

In actual plant operation in Duisburg, Fraunhofer ISE achieved a 39 percent increase in methanol production (using hydrogen and blast furnace gas) by adjusting the reactor inlet temperatures, the recycle ratio, and the hydrogen blend.

“The work conducted by Fraunhofer ISE enables simulation scenarios for a range of conditions: partial-load operation of a plant, scaling up to the next production capacity level, and fluctuating production conditions,” concludes Dr. Matthias Krüger from project partner thyssenkrupp Uhde. “Digital twins are particularly important tools for understanding and optimizing catalysts and process technology, especially for Power-to-X processes with fluctuating input conditions,” explains Dr. Andreas Geisbauer from project partner Clariant.

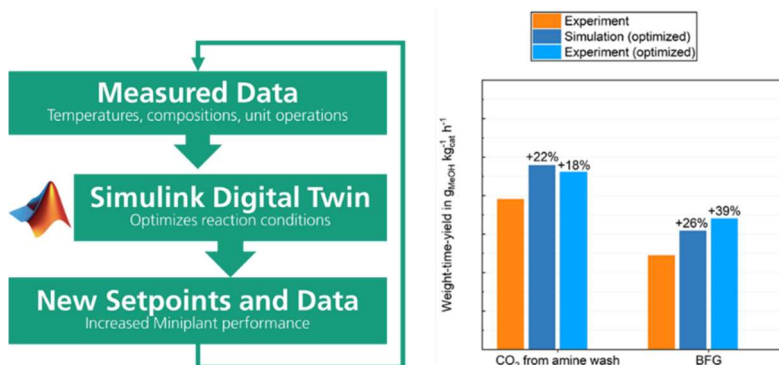
The Carbon2Chem® project is funded by the Federal Ministry of Research, Technology, and Space (BMFTR) and is currently in its third funding phase. Fraunhofer ISE was involved in the first two phases and laid the foundation for a successful Phase 3.

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Mini-plant for converting blast furnace gas into methanol. © Fraunhofer ISE



The simulation, based on real measurement data, suggested changes to the operating parameters. This made it possible to produce 39 percent more methanol from blast furnace gas (BFG) and hydrogen. © Fraunhofer ISE

More information: <https://www.ise.fraunhofer.de/de/forschungsprojekte/carbon2chem-phase-2.html>