Press release

Evonik Oxeno introduces AI-based process optimization into live plant operations

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- **AI-powered models translate insights from process simulations into plant control**
- **Initial applications improve energy efficiency and reduce CO_2 emissions**
- **The scientifically published methodology can be applied to additional chemical processes**

Marl, Germany und Antwerp, Belgium. Evonik Oxeno has introduced AI-based process models into live plant operations for the first time, achieving higher energy efficiency and lower CO_2 emissions. In addition, decisions can be made more quickly when changes in feedstock streams occur. The models were developed as part of the COMPAS project, short for Control and Optimization using AI Models for Process Advancement and Cost Saving.

Not all processes inside a chemical production plant can be directly observed, and the most efficient way to operate a production facility depends on numerous influencing factors. Conventional process simulations can provide valuable insights, but they are complex and time-consuming. To address this challenge, the COMPAS team developed an approach based on pre-calculated data. More than one million simulations of plant operating conditions provide the foundation for so-called gray-box models, which describe the plant's thermodynamics and kinetics through specially programmed and trained AI models. This enables COMPAS to draw on a comprehensive library of previously calculated scenarios and generate realistic recommendations for plant control within seconds.

“We combine our extensive knowledge of chemical processes with the capabilities of artificial intelligence. This allows us to bring complex process simulations directly into plant operations and support efficient plant control even under changing operating

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conditions," says Dr. Niklas Paul, Head of Engineering at Evonik Oxeno.

The technology is already being used in live operations in Marl and Antwerp. Current applications show a very high level of agreement between the models and actual operating data, enabling further optimization of plant operations. As a result, the energy consumption required to manufacture the desired product is minimized, directly improving the carbon footprint. Additional applications are already being implemented. These also include the automated transfer of results generated by the AI models to the plant control system.

"COMPAS demonstrates that the knowledge jointly built by operations, engineering and research over many years creates new value in process optimization through artificial intelligence. Based on this technology, we are working step by step toward a self-optimizing C4 Verbund," says Prof. Dr. Robert Franke, Head of Simulation & Kinetics at Evonik Oxeno.

The project team has also published the COMPAS methodology and recent findings in scientific publications in the journals "Chemie Ingenieur Technik" and "Chemical Engineering & Technology." The approach is not limited to the current applications at Evonik Oxeno. The methodology has the potential to be transferred to additional chemical and petrochemical production processes. The project team is continuing to expand the application scope of COMPAS and is seeking patent protection for the technology.

Link to the publication „Can AI-Based Surrogate Models Offer Added Value for Process Optimization? – Investigations Into Practical Application Examples in the C4 Verbund" published in "Chemical Engineering & Technology":
https://onlinelibrary.wiley.com/doi/10.1002/ceat.70291

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About Evonik Oxeno
Evonik Oxeno, a wholly-owned subsidiary of Evonik, is a leading company in C4 chemistry with 50 years of experience, operating two world-scale C4 production facilities in Marl and Antwerp. The flexibility of its integrated network allows Oxeno to quickly and efficiently respond to changing conditions in supply and demand, optimizing the complexity of value chains also for its suppliers and customers. Oxeno is recognized for its focus on innovation and sustainability, maintaining an impressive portfolio of approximately 2,100 patents and patent applications. Its C4 strategy is based on a solid foundation and defined measures for growth and transformation. The company's vision, "Chemistry4Future® – We increase the value of C4 chemicals sustainably," outlines its long-term goal and provides a clear idea of where it aims to see its business in the future.

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