

LANXESS planning AI-assisted formulation development for Urethane Systems

- **Platform for artificial intelligence to accelerate development of custom-made formulations**
- **Initial project phase successfully completed**

Cologne – LANXESS is broadening its use of artificial intelligence (AI) in product development. The specialty chemicals company has launched a project aimed at expanding its range of prepolymers. The goal is to offer customers tailor-made polyurethane systems with even shorter lead times, including for entirely new applications with different requirements. The Urethane Systems business unit is using the potential of AI and has brought materials AI company Citrine Informatics on board as a project partner.

In an initial project phase, LANXESS enlarged its database of prepolymer-based formulations. LANXESS data specialists and process experts used the Citrine Platform for artificial intelligence to add further data points to the company's formulation database. This involved linking existing empirical measurement data with the knowledge of the process experts and a chemistry-aware algorithm to calculate additional measurement values. This meant that only a few real-life measurements were required to verify the figures determined with AI.

In a next step, data and process experts at LANXESS will check how reliably optimal formulations can be predicted with the aid of AI to meet customer-specific requirements for product characteristics. "If the next tests are successful, we will be able to fulfill customer requests even more quickly and effectively. Our existing knowledge of formulations shall be enhanced by AI-assisted formulation design – in other words, systems that are not yet part of our portfolio but for which artificial intelligence will enable us to know instantly whether

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we can manufacture them and how,” says Markus Eckert, head of the Urethane Systems business unit at LANXESS.

AI complements domain knowledge

So far, chemists have largely had to rely on their specialist expertise and years of experience when researching new formulations with defined product characteristics such as hardness, tensile strength and viscosity. AI is expected to become an important tool to help them broaden their knowledge and significantly reduce the amount of tests required.

LANXESS already has some experience in using AI. In a pilot project with Citrine Informatics, the specialty chemicals company is using AI to optimize glass fibers as a way of further enhancing the properties of LANXESS high-performance plastics. It is anticipated that AI will cut development times for the necessary formulations by more than half. Customers will receive even better, tailor-made products within shorter time frames.

For Jörg Hellwig, Head of the LANXESS Digitalization Initiative, the partnership between Citrine and the LANXESS Urethane Systems business unit demonstrates the growing role of digitalization in product development. “Most employees who are already using artificial intelligence cannot imagine ever going back to the old methods of working. The use of digital technologies is increasingly becoming standard procedure at LANXESS,” says Hellwig.

Digitalization along the entire value chain

LANXESS launched its digitalization initiative in 2017 and established a dedicated team to handle it. It is headed by Chief Digital Officer Jörg Hellwig, who reports directly to Matthias Zachert, Chairman of the Board of Management at LANXESS AG. The initiative’s core fields of action are to develop digital business models, introduce new

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technologies along the value chain, develop and utilize big data and foster digital expertise among employees.

Citrine Informatics is the industry leader in the use of data and AI to accelerate the development of materials and chemicals. Citrine has been recognized for technology innovation by the World Economic Forum as a Tech Pioneer, and collaborates with some of the best universities in the world, including Carnegie Mellon University in Pittsburgh, Pennsylvania, and the University of California, Berkeley.

LANXESS is a leading specialty chemicals company with sales of EUR 7.2 billion in 2018. The company currently has about 15,400 employees in 33 countries and is represented at 60 production sites worldwide. The core business of LANXESS is the development, manufacturing and marketing of chemical intermediates, additives, specialty chemicals and plastics. LANXESS is listed in the leading sustainability indices Dow Jones Sustainability Index (DJSI World and Europe) and FTSE4Good.

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Forward-Looking Statements

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Information for editors:

All LANXESS news releases and their accompanying photos can be found at <http://press.lanxess.com>. Recent photos of the Board of Management and other LANXESS image material are available at <http://photos.lanxess.com>.

You can find further information concerning LANXESS chemistry in our WebMagazine at <http://webmagazine.lanxess.com>.

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Image



LANXESS develops numerous prepolymers for a wide range of polyurethane applications, such as star wheels for material separation and material transport. The use of artificial intelligence is expected to speed up the process of developing custom-made formulations for prepolymers. Tests are currently being conducted at the research and development laboratory in Naugatuck, U.S.

Photo: LANXESS AG

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