

Interview

with Dr. Steffen Kanzler*

A conversation about artificial intelligence at Evonik

What are current topics and trends in the chemical industry?

Thanks for having me. So far 2024 has been another challenging year. We saw a lot of supply chain disruptions and several players were facing production issues. Additionally, competition in Europe was highly active and many Asian players seem to have taken an interest in the European market. Volatility of energy costs and changing regulations and policies led many chemical companies to reevaluate their assets and production plant setups.

From our customers perspective, sustainability and circular economy principles have gained importance. We recently conducted a survey among our customers, and it clearly showed that sustainability will be a key topic for this year and going forward. Providing information on product carbon footprints, life cycle analysis or bio-based content in our products has become an opportunity to differentiate yourself from competition. Many customers have sustainability scorecards for their suppliers and manage their business to a certain degree according to their sustainability scores. Evonik is a pioneer in this area. We aspire to create sustainable, value-added solutions for our customers. Evonik has integrated sustainability into the corporate strategy, from research & development through portfolio management to corporate culture. Our goal is to increase the share of our portfolio with strong positive sustainability profiles to over 50% by 2030, today we are at about 43%.

Evonik has also committed to support the objectives of the Paris Agreement on Climate Change. For instance, Evonik commits to the Science Based Targets initiative (SBTi) and aims to reduce our scope 1 and 2 emissions by 25 percent, while scope 3 emissions are targeted to be reduced by -11%. All this is in line with the SBTi target level of "well below 2°C". Another key topic for 2024, and probably for the coming years, is digitalization and artificial intelligence. I see a lot of activity in this area by many chemical companies. Data has become important across all our businesses; it is almost like a new feedstock for us. Here as well Evonik is an early adaptor, digitalization and AI are key elements of our strategy and Evonik has been actively looking at AI and its application within the chemical industry for many years now.

How do you see artificial intelligence impacting the chemical industry in the next 5-10 years?

We see artificial intelligence having a significant impact on our industry in the next 5-10 years. There is potential for benefits of AI in the automation of standard manual tasks in customer service and supply chain, such as order intake, no touch orders, forecasting, or production planning optimization. AI can definitely help here; however, I see it rather being a tool that complements humans or frees up their time for other tasks such as direct customer communication. AI is usually good when there is a lot of data and high quality in the data,

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with limited bias. For this application usually prerequisites for a successful implementation of AI are met.

In addition to these areas, we see a use case for AI for innovation in the chemical industry. For instance, AI can be used to screen for new molecules and predict their properties, which saves us time and cost for testing, and it may allow us to speed up the development of new products and bring them to market faster. There are large databases of molecule properties available with which one could train AI and then predict the behavior of new molecules, e.g. for finding new hardeners for coatings that deliver great heat resistance or chemical resistance properties. I have seen already some academic publications in this area where AI accurately predicted molecule properties, in the future this could be a game changer for the chemical industry, innovation is key for any specialty chemical company, and it is cost and time intensive. Thus, any help of AI in this area is highly welcome.

Other areas where we see potential for AI in the chemical industry include process optimization, quality control, and predictive maintenance. By using AI to analyze data from sensors and other sources, we can identify potential issues in production before they occur and take corrective action to prevent downtime and improve product quality. Predictive maintenance is a keyword here and for accident prevention I can see that AI could be very useful in the future. AI could be trained with various data from production plants sensors on "close calls, or prevented incidents" as well as actual production accidents and plant failures and then this AI could be used to predict future cases and help to prevent those.

Overall, I believe that the use of AI in the chemical industry will continue to grow, and we will see more applications emerge in the coming years. This technology has the potential to transform our industry and help us stay competitive in an increasingly complex and challenging market.

Before we continue in to detail with AI; many of our readers are currently studying business chemistry and you are a business chemist working currently in an interdisciplinary position, tell us a bit about your career?

I joined Evonik in 2012 after completing my PhD and I took over a project manager role, which was similar to an inhouse consulting role. After about two years in that role, I joined the business line Crosslinkers and more specific their new

business development group, where I was responsible for composite applications of our amine hardeners. Then, I had the opportunity to move to the USA as a business development manager for North America and sales rep for Mexico. During my time in the US, Evonik offered me a marketing position, and from 2017 on I was in charge of marketing for the market segments Adhesives and Composites. At the end of 2020 after about 4.5 years in the US, I moved back to Germany and joined the business line High Performance Polymers, here I held a marketing position for our Vestakeep® products, with a focus on automotive and aerospace applications. After two years in this role, I was offered a marketing director position back at the business line Crosslinkers, which I happily accepted. Here I am responsible for our Coatings business in EMEA. Furthermore, we are working on a lot of projects regarding digitalization. Evonik is also looking into different trending topics, including future applications of AI in the chemical industry.

Can you provide an example of how your company is currently using AI to improve efficiency or productivity in the chemical manufacturing process?

Yes, there are a couple of projects and applications that I can name here. Actually, Evonik sees itself as a pioneer for digitalization and the application of AI in the chemical industry. For instance, we are the first chemical company to participate at the MIT-IBM Watson AI Lab based on the MIT campus in Cambridge, Massachusetts. Experts from academia and industry are working together to better understand AI and its application potential for the chemical industry among other topics. Here research is done on AI supported material discovery, formulation technology, knowledge management, market analysis and more in general on decision making, e.g. how AI can help to make better and faster decisions. We have an active partnership with IBM on topics like this since 2017 and we have completed several projects, i.e. our scientists no longer have to search for expert knowledge like for a needle in a haystack. Instead, decades of knowledge and information are now easy to search and to analyze intuitively with support of AI, our chemists can easily explore and compare formulations and their related properties to come up with new developments and innovative products.

One of our AI applications is COATINO®, our virtual formulation assistant, which is available free of charge

to the entire paint & coatings industry. Coatings and paint formulators can go on our webpage www.coatino.com and can request AI-based additive recommendations for their specific applications, for example with individual guiding formulations for pigment concentrates. The AI application COATINO® now can even be used via voice control. The recommendations by COATINO® and its algorithms rely on both AI-based technology and machine learning principles. Evonik operates a high-throughput equipment that tests and evaluates up to 120 coating formulations per day and feeds these results into the continuous improvement of COATINO®. Besides large amounts of data the AI tool is of course also enriched by years and years of experience of Evonik's additive experts. When using COATINO® formulators can select from over 200 product properties and effects to obtain tailor-made and weighted recommendations. In theory 1070 property combinations are possible, and the tool includes around 1,900 existing and tested guiding formulations. Additionally, COATINO® can calculate individual formulations for all types of pigment concentrates and the data pool it is basing the recommendations on is constantly growing. Many of our clients really appreciate the voice command option, because, if unexpected challenges arise in the laboratory, technicians and scientists can obtain technical information on additives and still have both hands free to continue their work in parallel.

A decisive factor in the development of COATINO® was the creation of maximum transparency for the customer. The recommended products can be dynamically compared with each other, so that the customer can grasp the differences in a few seconds and thus make their decision. A total of almost 300 products are available to choose from, including defoamers, dispersing additives, and matting agents. COATINO® sends out all technical, regulatory, and safety data sheets conveniently via the watch list if required.

Another application of AI at Evonik is the SciTai which stands for Scientific Technical Support by AI, one of first projects that was initiated as part of the strategic partnership with IBM. This AI tool helps Evonik compound experts to get easier access to the accumulated knowledge of internal research results via an intelligent graph database, consisting of over one million nodes connected with over 14 million links. The result of this lighthouse project is a knowledge platform with logically linked information from various sources, that represent over 20 years of research, digitally available in one central place. SciTai also has the capability to predict material properties and can give formulation recommendations based on AI.

Finally, I want to mention our self-learning Market Intelligence Platform CRISP (Cognitive Raw Materials Intelligence Service Platform) at Evonik Procurement. The idea for this AI application emerged in 2016, when it became more and more clear that the growing quantity of digital information on raw material prices, different indices, market volatilities and emerging and disappearing players made evaluation by humans very time consuming and difficult. Instead of having sourcing managers do the market research themselves e.g. going on a hunt for information, the idea was that the relevant information should come to them with the help of AI. For that the AI searches news sites from around the world, social media and market reports, after that CRISP autonomously selects the relevant information and then provides the information to the user in form of a personalized newsfeed, these reports will then be evaluated by our sourcing managers of which the AI then learns for future reports. In multiple cases our users of CRISP report that the AI recommended them information that turned out as highly relevant, which they would not have found without the AI, e.g. in one case CRISP recommended an article from a foreign newspaper that mentioned an event which was a key piece of information in refining a sourcing strategy for a certain raw material. In sourcing speed is of the essence and early warning signs on supply disruptions due to incidents at suppliers or transportation route disruptions often are first discussed on social media before they are picked up by traditional news channels. CRISP picks those up and helps our sourcing managers to get a head start in reacting to sudden changes.

How do you ensure the accuracy and reliability of AI-generated data in your operations?

Evonik ensures the accuracy and reliability of AI-generated data in our operations by following a rigorous process. First, we carefully select and curate high-quality data that is relevant to the specific task at hand. We then use validation techniques such as comparing the AI-generated data to original true data or using statistical methods to ensure that the data is accurate and reliable. Once the AI model is deployed, we monitor its performance using automated monitoring systems and regularly review its output to ensure that it continues to generate accurate and reliable results. We also continuously improve the AI model by retraining it on new data and fine-tuning its parameters to ensure that it remains accurate and reliable with time. In addition, we

have a team of experts who are responsible for overseeing the AI-generated data and ensuring that it meets our high standards for accuracy and reliability. This team works closely with our data scientists and engineers to ensure that the AI-generated data is used effectively in our operations and that any issues are quickly identified and addressed.

What challenges have you faced in implementing AI technology in the chemical industry, and how have you addressed them?

We have faced several challenges in implementing AI technology. One major challenge is the data quality and availability. We have a lot of data, but it is often scattered across different systems, and the quality of the data may not be sufficient for training AI models in some cases. To address this, we have invested in systems and processes to ensure that data is properly collected, stored, and maintained. We have also explored partnerships with data providers and other companies to access additional data sources, and of course we collaborate with AI experts, like the MIT-IBM Watson AI Lab, which I mentioned earlier.

Another major challenge are regulatory concerns. The chemical industry is heavily regulated, and there may be concerns about how AI technology will impact compliance with regulations. To address this, we have worked closely with regulatory bodies to ensure that our AI systems comply with all relevant regulations and guidelines, and we continuously work here to be compliant.

Additionally, Evonik has invested in personnel that has the necessary knowledge for employing AI in the chemical industry. Evonik has hired data scientists, engineers, and other AI experts and we have also partnered with AI service providers and other companies to access specialized expertise, for instance regarding chatbot technologies.

Finally, the implementation of AI technologies required significant changes to existing processes and workflows, which sometimes can lead to skepticism from employees or customers. To address this, we have invested in change management processes and communicated the benefits of AI technology to employees and customers, and we are providing a lot of training opportunities. We have also involved employees in the implementation process to ensure that their concerns and feedback are addressed.

Overall, we recognized early that implementing AI technology in the chemical industry requires significant investment and effort. However, we believe that the benefits of AI technology, including improved efficiency and safety, and potentially also

for sustainability, make it a worthwhile investment for our company and the industry as a whole.

How do you balance the potential benefits with the risks of AI in the chemical industry?

At Evonik we of course also recognize the risks associated with AI. One of the most significant risks of AI is „garbage in, garbage out“. This occurs when the quality of the data used to train the AI model is poor, resulting in inaccurate predictions and maybe wrong decisions. Therefore, data quality is always one of our main criteria when we start to train an AI model for a project. AI algorithms rely heavily on large data set, but also on high quality data, and if the data is incomplete, inconsistent, or inaccurate, it can lead to incorrect problems that one might notice only after a while. We always try to have processes in place to identify and correct any data quality issues, which sometimes is difficult because what the AI actually does is often kind of a black box. Thus, we work with experts to get transparency on the inner workings of our AI algorithms.

Bias is another significant risk associated with AI. AI algorithms can be biased if they are trained on data that is biased, or if the algorithm itself has inherent biases. We work hard to ensure that the data used to train the AI model is free of biases. Everybody in the AI field knows about the case at Amazon in 2018, when they shut down their AI recruiting tool, after realizing that it was discriminating against women. Incidents like that, we try to avoid from the start of course. Additionally, we regularly monitor and audit our AI systems to identify and correct any biases that might occur.

Overall, in balancing the potential benefits with the risks of AI in the chemical industry, we always prioritize safety and quality. Evonik ensures that any AI system that gets implemented is thoroughly tested and validated by our experts before it is used. I am looking forward to many additional applications and use cases of AI within Evonik, for the chemical industry the benefits can be huge and I feel we are still in the early phases of the adaption of this new technology and there is much more to come.