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Commentary

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How artificial intelligence can be used in the chemical industry

Introduction

The chemical industry is discovering more and more opportunities to leverage the power of artificial intelligence (AI). Although AI as an active scientific discipline is around since the 1950s (Wooldridge, 2018) and has gone through several waves, it now seems to be on the radar of almost every chemical company. While the integration of AI in chemical engineering is not novel, its comprehensive application and potential are yet to be fully realized (Venkatasubramanian, 2019). Energy and oil price volatility as well as supply and demand fluctuation force the chemical industry to be more agile in order to adapt faster to this new market environment. Additionally, stakeholders on all sides expect significant efforts regarding environmental responsibility, sustainability and circularity. Furthermore, innovation is a key driver of competitive advantage and differentiation in the chemical industry, however with more stringent regulations and pressure on innovation budgets, identifying and then speeding up the most promising R&D projects is more important than ever. Hence, AI is a critical tool in the transformation the chemical industry is facing.

According to a recent survey conducted by IBM (Womack et al., 2020), an 80% of managers within the chemical industry acknowledge the imminent transformative influence of artificial intelligence on their business operations within the next three years. This statistic underscores the industry's recognition of AI as a pivotal driver of change, signaling a paradigm shift in how chemical companies operate and innovate. The survey further describes major areas where AI is anticipated to make significant inroads, with research and development leading at 74%, followed by production optimization at 61%. Additionally, AI is expected to play a pivotal role in forecasting and planning, with 47% of respondents identifying it as a critical area for AI implementation. Moreover, risk management emerges as another focal point for AI integration, with 58% of surveyed managers recognizing its potential to enhance decision-making processes and mitigate operational risks (Womack et al., 2020). To summarize recent activities this commentary will explore key areas for AI application within the chemical industry.

AI applications in the chemical industry

Ensuring safety remains paramount in chemical manufacturing, where the repercussions of accidents can be catastrophic. AI offers a transformative solution by leveraging predictive analytics to anticipate potential hazards and preemptively mitigate risks. Machine learning algorithms, particularly supervised learning models, are well-suited for this task. For instance, AI systems can analyze historical data to identify patterns indicative of impending accidents, enabling proactive intervention (Mao et al., 2019). Similar to the use of AI, for instance in the radiology space, where the AI was trained with images of abnormalities from diagnostic scans and can now help to improve diagnostic accuracy and also reduce the radiologists workload (Giansanti et al., 2021; Kelly et al., 2022; Mun et al., 2020), AI in the chemical industry could be trained with critical production plant data before accidents had happened in the past, to better predict failures in the future. Furthermore, AI can revolutionize safety training by providing immersive virtual reality experiences that simulate hazardous scenarios. Today AI-driven simulations can facilitate virtual testing of safety protocols and emergency response strategies, and augmented reality is used to prepare the workforce and helps minimizing the likelihood of incidents (Chiang et al., 2022). By continuously adapting to evolving safety standards and regulations, AI-driven training

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modules ensure that employees in the chemical industry are up to date with best practices and protocols.

As the IBM survey demonstrates, AI has found its way into R&D and innovation departments. AI's capacity to analyze vast datasets unlocks unprecedented avenues for innovation in molecule design. Through machine learning algorithms, researchers can expedite the discovery of eco-friendly materials and chemicals, thereby avoiding the reliance on conventional, environmentally harmful substances (Schmidt et al., 2017). For instance, AI-driven simulations enable virtual screening of molecular structures, identifying compounds with desirable properties for various applications. This approach not only accelerates the development of new products but can also minimize the environmental footprint associated with traditional synthesis methods. Deep learning algorithms, particularly generative models, hold promise for material design tasks. For example, generative adversarial networks (GANs) can generate novel molecular structures with desired properties by learning from existing chemical data. Real-life applications include the use of GANs to design organic photovoltaic materials with improved efficiency and stability, accelerating the development of renewable energy technologies. By leveraging machine learning algorithms, researchers can expedite the discovery of novel catalysts and reaction pathways, thereby enabling also the development of greener synthesis methods (Doan et al., 2020). Through AI-driven simulations, scientists can better predict molecular interactions, revolutionizing the way new materials and compounds are designed and synthesized. Furthermore, AI-driven synthesis holds promise for decentralized manufacturing and on-demand production, offering a pathway to reducing reliance on centralized facilities and transportation networks. By integrating AI into small-scale reactors and production units, chemical manufacturers can customize processes to meet localized demand while minimizing environmental impact.

Additionally, AI is driving innovation in the field of green chemistry, where the emphasis is on designing processes that minimize or eliminate the use and generation of hazardous substances. Through AI-enabled predictive modeling, researchers can identify reaction conditions and solvent systems that maximize yield while minimizing waste and energy consumption. For example, AI algorithms can analyze reaction databases to identify sustainable alternatives to traditional solvents and reagents, leading to more efficient and environmentally friendly synthesis routes. Moreover, AI is facilitating the development of autonomous chemical synthesis platforms, where robotic systems can perform complex synthesis tasks with minimal human intervention. These platforms leverage AI algorithms to plan and execute synthesis routes, monitor reaction progress in real-time. However, those applications are still rather in the future. According to Walter Grüner, Head of IT & Digitalization at Covestro: "[...] the chemical industry is predestined for the use of AI because we have a lot of complex processes going on that cannot be described by fixed rules. They are not suitable for automation. We rather need learning systems to which we grant a certain degree of decision-making autonomy. In doing so, we focus primarily on the development of systems that work in a complementary manner to humans and support their abilities." (Rothbarth & Weiße, 2023).

However, when AI complements chemical engineers very often process optimization are the result. By harnessing AI-driven predictive modeling with human supervision chemical plants can dynamically adjust process parameters in real-time, optimize energy consumption and resource utilization (Shinkevich et al., 2021). Moreover, AI-enabled process monitoring facilitates early detection of inefficiencies, allowing for timely intervention and continuous improvements. Machine learning techniques, such as reinforcement learning, are particularly well-suited for process optimization tasks. For example, AI systems can learn optimal process control strategies by accessing historical data complemented by input from experienced plant engineers. Through iterative learning, these systems then can adapt and refine control protocols to maximize energy efficiency and minimize waste generation. Real-life examples include the use of reinforcement learning algorithms to optimize reactor operations in chemical plants, leading to significant reductions in energy consumption and production costs (Shinkevich et al., 2021).

For example in 2021 in Japan 20 chemical companies started to collaborate on the development of an AI based system to shorten development times on new durable and heat-resistant materials. The companies share their data and also extract training data from patent databases. In doing so they expect to reduce development times from decades down to several months (Goto, 2020). The AI powered approach again complements traditional development

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methods which relied on researchers' experience along with educated guesses or trial and error.

Another area were AI will play an important role for the chemical industry is supply chain optimization.
Efficient supply chain management is instrumental in minimizing the waste of resources in the highly complex chemical industry. AI-driven analytics offer support by optimizing inventory management, transportation logistics, and demand forecasting. By analyzing historical data and market trends, AI systems can predict demand fluctuations with high accuracy, enabling proactive inventory replenishment and minimizing stockouts (Chiang et al., 2022). Predictive analytics techniques, such as time series forecasting and anomaly detection, are well-suited for supply chain optimization tasks. For example, AI systems can analyze historical sales data to forecast future demand patterns and optimize inventory levels accordingly. Additionally, anomaly detection algorithms can identify deviations from expected supply chain behavior, allowing for proactive risk mitigation and contingency planning. Real-life examples include the use of predictive analytics to optimize inventory management in chemical supply chains, reducing carrying costs and improving overall efficiency. Furthermore, AI-powered routing algorithms optimize transportation routes, reducing fuel consumption and emissions associated with product distribution and AI can help by including weather data with operational data to adjust routing, and lead times (Womack et al., 2020).

Some 81% of companies surveyed by IBM, which they call AI champions also started to include AI to improve the customer experience. For instance Evonik has launched COATINO a virtual assistant that can help coating and paint formulators with recommendations on which coating additives to use or what pigment concentrations are best for a specific customer application (Womack et al., 2020). Other companies started to use AI in the customer service department, e.g. by automating order intake via AI, with the goal to achieve zero-touch orders, i.e. human actions required to complete an order from order-in-take until invoicing are reduced to near zero. This frees up resources for more value generating tasks.

Conclusion

In conclusion, AI will be a powerful tool for the chemical industry. However, AI also comes with risks. While the integration of AI holds immense promise for driving sustainability within the chemical industry, several challenges must be addressed to realize its full potential. Firstly, the development of AI-driven solutions requires interdisciplinary collaboration between industry stakeholders, academia, and government agencies. This collaboration is essential for leveraging diverse expertise and resources to tackle the complexities of the chemical industry. Secondly, concerns regarding data privacy, security, and ethical considerations will require robust regulatory frameworks to ensure responsible AI deployment (Venkatasubramanian, 2019). As AI technologies become more pervasive in chemical manufacturing, it is essential to establish clear guidelines and standards for data collection, sharing, and usage to protect intellectual property and ensure compliance with regulatory requirements. Moreover, continued investments in research and development are imperative to enhance AI capabilities and tailor them to the unique needs of the chemical industry. This includes advancing fundamental research in AI algorithms and techniques, developing specialized AI tools and platforms for chemical applications, and providing training and education to empower the workforce to harness the full potential of AI-driven technologies. In conclusion, Artificial Intelligence stands as a powerful catalyst for the chemical industry. By harnessing AI-driven technologies, we can optimize processes, create safer work environments, speed up innovation, streamline supply chains and help facing the challenges of the chemical industry. As AI capabilities continue to improve, the potential for innovation and sustainability could be immense and I am looking forward to seeing these developments.

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