SCIENTIFIC PAPERS OF SILESIAN UNIVERSITY OF TECHNOLOGY ORGANIZATION AND MANAGEMENT SERIES NO. 172

ARTIFICIAL INTELLIGENCE IN THE CHEMICAL INDUSTRY – RISKS AND OPPORTUNITIES

Mateusz LASKA^{1*}, Izabela KARWALA²

¹ Grupa Azoty S.A.; mateusz.laska@grupaazoty.com, ORCID: 0000-0003-0124-3496
² Grupa Azoty S.A.; Akademia WSB; izabela.karwala@doktorant.wsb.edu.pl, ORCID: 0000-0003-0991-7301
* Correspondence author

Purpose: The aim of the article is to review the literature on the risks and opportunities of implementing Industry 4.0 - Artificial Intelligence solutions in the chemical industry.

Design/methodology/approach: The review was carried out using available scientific articles, popular science publications, and media reports from the world's largest companies in the chemical industry.

Findings: The analysis indicates that there are more benefits than risks arising from the implementation of Artificial Intelligence solutions in the chemical industry.

Research limitations/implications: The frequent lack of specific economic indicators makes it difficult to clearly indicate the implementation potential of a specific solution in other companies in the chemical industry.

Social implications: The implementation of AI in chemical industry companies can reduce environmental pollution, raw material consumption, and optimize production processes.

Originality/value: The article, based on real data, is aimed at middle and senior management of companies in the chemical industry, presenting the advantages and disadvantages of implementing AI solutions in the chemical industry.

Keywords: AI, Chemical Industry, Machine Learning, Risks, Opportunities.

Category of the paper: Literature review.

1. Introduction

Over 80% of managers in the chemical industry surveyed by IBM admit that artificial intelligence (AI) is going to have a huge impact on their business within the next three years. The areas in which AI is most commonly implemented in this sector are research and development (74%), production (61%), forecasting and planning (47%), and risk management (58%) (Lin et al., 2020). According to a survey conducted by Accenture (Accenture, 2014), 94% of managerial staff in the chemical and advanced materials industry expect the digitization

of the entire industry, and AI plays a crucial role in enabling the digital revolution (World Economic Forum, 2017). The latest technologies allow chemical companies to reduce operating costs, increase profits, and improve product quality. The chemical industry is increasingly interested in using AI to solve problems related to process modelling, optimization, control, as well as fault detection and diagnosis (Hajjar et al., 2016). This article reviews the methods of applying AI in the chemical industry and examines its potential for the sector.

2. AI applications in the chemical industry

The industrial sector has a significant impact on the global economy in the long term. In 2022, the size of the global chemicals market was valued at USD 616 billion. It is forecasted that this value will achieve an annual growth rate of 5.1% by 2030. However, recent events such as the outbreak of the Covid-19 pandemic and geopolitical tensions have had a negative impact on the development of this sector. Unstable energy prices, higher production costs, temporary closure of production plants, and numerous disruptions in the value chain of specialized chemicals have resulted in a periodic decline in production and demand (Market Analysis Report, 2022). The significance of the manufacturing sector for economic growth goes beyond direct production. The development of the industry translates into growth in other sectors of the economy, including job creation. A stable industry plays a crucial role, especially in situations of international trade downturns. Indeed, having a robust industrial sector helps to maintain economic security during crises (Development and Technology Ministry statement).

The recent climate, economic, and social changes have had an impact on the future of the global economy. Companies are focusing on efficient innovation acquisition and implementation to achieve defined goals in response to emerging challenges. In a report prepared by Innogy (2019), the authors identified three main megatrends that they believe will shape the future of the industrial sector. These include digital, climate, and organizational transformations. These areas have been singled out due to their relevance, universality, and multifaceted nature. One of the biggest challenges facing contemporary chemical companies is digital transformation. The current socio-economic situation makes it a sort of a business ultimatum, determining the survival of organizations in the market (Matt, Hess, Benlian, 2015). Due to its specificity, the chemical industry is characterized by a high degree of process automation.

Continuous investment in the development of innovative technologies is essential for companies to grow. One of the most rapidly developing fields is the artificial intelligence system and its application in production processes. According to the OECD, artificial intelligence is a machine-based system that influences the environment by formulating recommendations and predictions using input data from machines and humans (OECD, 2018).

In reports prepared by the European Commission, AI is defined as software systems designed and improved by humans, operating in a physical or digital dimension, collecting and analysing data to predict actions necessary to achieve a set goal. Analysing the concept of AI from the perspective of scientific disciplines, it covers areas such as machine learning (including deep and reinforcement learning), machine reasoning (referring to planning processes, knowledge implementation, search, optimization), as well as robotics (including control, perception, sensors, actuators, and the integration of other techniques used into cyber-physical systems). In practice, building an AI system is mainly done through machine learning. Intelligent devices, based on conclusions drawn from previous experiences, using a neural network composed of algorithmic networks, search for connections between variables and process accumulated data in a way that is similar to the human brain. Given the multitude of AI applications and the enormous potential associated with its widespread use, it is impossible not to appreciate the role it plays in the chemical industry. Figure 1 presents the main areas of chemical production where AI has found its application.

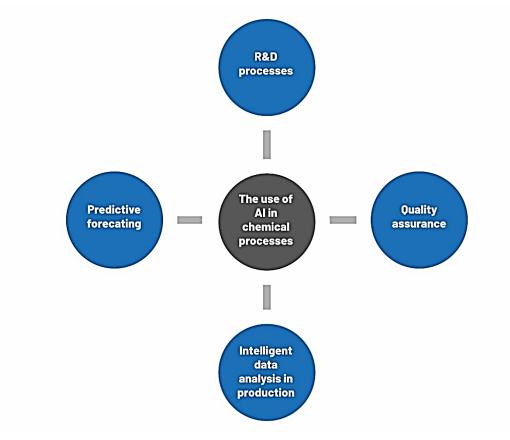


Figure 1. Examples of AI utilization in chemical processes. Source: Own elaboration.

2.1. Solutions using artificial intelligence for research and development processes

Research and development play a fundamental role in industrial innovation, especially for companies related to sustainable development (Hájek, Stejskal, 2018). Artificial intelligence is used to predict and optimize chemical reactions (Marcou et al., 2015; Mohammadi, Penlidis, 2018; Zhou et al., 2017) and to improve the design of chemical synthesis (Segler et al., 2018). Machine learning has been investigated for screening research and catalyst design (Li et al., 2017; Li et al., 2017; Zahrt et al., 2019). Several studies have highlighted the potential of artificial intelligence in supporting the development of sustainable chemicals and materials (Doan et al., 2020; Gu et al., 2019). In addition to these technical aspects, one study examined the use of artificial neural networks to assess and improve job satisfaction in research laboratories (Azadeh et al., 2015).

2.2. Predictive Forecasting

Machine learning and artificial intelligence models, along with advanced analytics, help to predict the amount of raw materials needed to ensure continuity in chemical production and to determine future demand. AI forecasting leaves room for changes at every stage of the molecule's development. Artificial intelligence also helps to predict the prices of materials and raw materials. This allows for faster adjustment of the production process to market conditions and significantly reduces the company's losses. Artificial intelligence used in the chemical industry can reduce forecasting error by 50% compared to human predictions. Companies can streamline their supply chain and avoid excess inventory by forecasting demand using artificial intelligence (McKinsey, 2017).

2.3. Intelligent data analysis in production

Companies operating on the market are obliged to comply with a number of regulatory standards. Exceeding the permissible values of carbon dioxide emissions, water consumption, or the level of pollution in production facilities results in a significant increase in costs. Manual control of indicators responsible for their regulation is very labour-intensive. For this reason, thanks to data analysis based on artificial intelligence, companies can easily track and adjust their production to standards introduced by state authorities. Moreover, with the progress of technology and the use of intelligent sensors, data analysis makes it possible to identify defects and inform employees about inconsistencies that have occurred. Knowing the source of the problem, experts can intervene in the production process and quickly solve the problem.

2.4. Quality Assurance in Production

In the chemical industry, timely quality assurance is of great importance. If an improper substance gets into the product line, it can cause irreparable damage, resulting in huge financial losses. With the help of artificial intelligence, it is possible to continuously monitor plant

operation and detect such cases, which ultimately helps to prevent equipment failures and production line downtime. Moreover, AI tools can learn from such incidents and use this knowledge to solve similar problems more effectively in the future. Quality assurance in chemical production is mainly ensured by computer vision. Using deep learning algorithms, computers scan substances on production lines, evaluate them, and classify them based on their properties.

3. AI Applications in the Chemical Industry

AI technologies are not a novelty in the chemical industry. For many years, they have been used by chemical companies around the world to develop products, forecast demand, and test quality. Here are some of the most popular examples of using artificial intelligence in the chemical industry.

3.1. AI-based production robots, cooperating and context-aware

Chemical companies use robots to clean production areas, minimizing human contact with toxic substances. Context-aware robots can also improve logistics efficiency and shorten travel time for raw materials or finished products between different parts of the production line.

Companies such as Novartis use robots to distribute chemicals on multi-well plates. They help the company test substances and products 24/7, accelerating the process of discovering new drugs.

3.2. AI in visual quality and safety control

Optical systems supporting artificial intelligence are used to detect defects such as mechanical inclusions, colour differences, or damaged packaging. AI platforms, such as SG Vision AI, provide advanced monitoring tools that help companies improve data collection accuracy and accelerate the model validation process (Pace, 2021).

Multi-billion-dollar companies such as Dow use AI monitoring to detect and eliminate safety threats associated with entries into enclosed spaces (Andulkar, 2021).

3.3. Algorithmic predictive forecasting in supply chain management using AI

Traditional forecasting systems are overwhelmed by the amount of data available on the internet. AI algorithms analyse huge amounts of data and predict demand for a specific product. Companies can adjust production planning and increase cost efficiency based on AI analysis results. In addition, they can implement artificial intelligence to collect data at sales points to predict customer demand and reduce waste associated with items that are not in demand.

Organizations such as Blue Yonder promote AI and machine learning techniques to optimize forecasting and inventory replenishment, while also having the ability to adjust prices simultaneously.

The supply chain is an integrated network in which different entities such as suppliers, manufacturers, and distributors work together to transform raw materials into finished products and deliver them to customers (Beamon, 1998). Artificial intelligence has been used to support the design, planning, and optimization of chemical supply chains, taking into account various environmental and economic aspects, for example: genetic algorithm (Berning et al., 2004; Guillén et al., 2006), heuristic algorithm (Pozo et al., 2012)). Some studies focused on supplier selection - for example, case-based reasoning (Zhao and Yu, 2011), while others used artificial intelligence techniques to predict and manage disruptive events, such as agent-based modelling (Behdani et al., 2009, 2012, 2019; Ehlen et al., 2014). Earlier research also included artificial intelligence in traditional modelling techniques for renewable materials supply chains, such as biomass (Castillo-Villar, 2014; Ghaderi et al., 2016; Lan et al., 2019).

3.4. Product property prediction

Japanese company Mitsui Chemicals has implemented technology for predicting the quality of reaction gases. It performs a real-time analysis of 51 different factors, including reactor conditions and process parameters. The new technology has enabled the company to improve the accuracy of reaction signals, resulting in safer and more stable operation of chemical plants. In the future, plant managers will be able to use deep machine learning to analyse huge amounts of data in real time, improving the accuracy of forecasts and control in operational processes, especially during start-up processes and modifications to increase production. It is also going to provide greater transparency in assessing the actual condition of machines and installation components and improve risk management effectiveness. AI-based tools enable production continuity, among other things, because machine learning more accurately predicts failures or the need for maintenance (Mitsui Chemicals, 2021)

BASF has applied a similar solution. In August 2019, they signed a cooperation agreement with Technische Universität Berlin to develop appropriate new mathematical models and algorithms for basic issues related to process chemistry and quantum chemistry.

Kebotix, an American technology platform that optimizes the production of new chemicals and materials using AI and robotics, has announced a strategic collaboration with Dutch company SCM, which specializes in precise methods for predicting properties through atomic modelling.

AI can be used in the area of creating new products. The goal set by Pfizer is to identify new and more precise treatment options by combining AI and data analysis with actual data. The company uses AI to redefine and accelerate the time it takes to complete chemical research (Kantify, 2023). Given that AI development technologies are still in the research phase, it can be assumed that in the coming years there will be a number of new benefits and applications arising from its implementation in the chemical industry.

4. How chemical companies use AI – threats and opportunities

The use of artificial intelligence (AI) by chemical companies is a natural consequence of their pursuit of Industry 4.0. It is undeniable that highly digitized companies can easily access a broad customer base worldwide, which translates into increased opportunities for scaling their business. The increase in the level of automation of production processes, digitalization, and modern machine and equipment stocks are key to increasing the resilience of enterprises to crises and changes in markets. The use of AI solutions in business processes is becoming increasingly common, and the range of applications and benefits arising from their implementation in production processes is generating greater interest among companies. For the vast majority, this is just the beginning of changes that will revolutionize the industry in the near future. On the other hand, the use of AI still raises a number of risks and controversies among employees. Table 1 presents the main advantages and disadvantages of using AI in production processes.

Table 1.

Category	ТҮРЕ	
	Chances	Threats
Economic	 savings resulting from process optimization increase in profits from sales, Preventing the accumulation of excess stocks 	 capital intensity uncertainty of return on investment,
Technical	increasing the efficiency of devices,improving product quality	 data security, vulnerability to cyberattacks,
Social	elimination of human errors,improving employee safety,	 fear of losing a job, protection of privacy, lack of specialist knowledge, ethical considerations
Environmental	 reduction of the number of post-production waste, lower energy consumption, a tool enabling the achievement of EZŁ objectives, 	• increasing the amount of carbon footprint
Research & Development	 accelerating innovation processes stimulating the development of new products and services 	• Dependence on technology

Pros and cons of AI applications in production processes

Source: own elaboration.

The use of AI algorithms by companies provides higher profits through operational optimization. AI-driven analyses of root causes and test procedures lead to waste reduction and product quality improvement. They stabilize flow and increase device efficiency. Moreover, organizations can adjust to different production variants using AI tools. They can also automatically control manifestation conditions, such as mixing speed, temperature, and process duration. Higher throughput and a 30% decrease in efficiency are possible. Another reason why the production sector is striving for digitization and automation is the profitability of AI solutions. Intelligent tools help companies increase sales and productivity by eliminating the possibility of human error. AI algorithms help analyse changing customer demand and optimize offerings. This is beneficial for achieving maximum profit and preventing excessive inventory. AI solutions can reduce sales and inventory losses by 65% and 50%, respectively.

Another area where AI has found application is environmental protection. In line with the idea of sustainable development, AI enables the creation of global climate models, precision agriculture development, and intelligent power grids to regulate energy consumption. AI also helps reduce waste, which is beneficial from an economic standpoint. According to Nature Communications, AI solutions enable organizations to be 63% more environmentally friendly (Vinuesa et al., 2020).

Artificial intelligence technologies, such as advanced analytics, real-time data collection, and the Industrial Internet of Things (IIoT), can help improve the safety of personnel and physical resources. AI tools prevent potential production-related hazards by eliminating the need for direct human involvement. By collecting data on-site, artificial intelligence significantly facilitates compliance with data collection and documentation requirements.

Currently, only 4 out of 10 chemical companies widely implement artificial intelligence in their operations. Slow progress related to the implementation of AI in production processes is due to several challenges facing this technology. They include, among others:

- underdeveloped tools,
- lack of AI skills among the workforce,
- lack of high-quality data,
- issues of trust and transparency,
- uncertainty regarding return on investment.

To minimize their negative effects, companies should prepare to incorporate AI into their business processes. It is necessary to have a clear understanding of the goals of AI implementation and specific areas where it is intended to be used. As technological progress continues, the benefits of using artificial intelligence in the chemical industry are beginning to outweigh the challenges of its implementation.

One of the main risks associated with artificial intelligence in the chemical industry is the possibility of human error. As artificial intelligence systems become increasingly sophisticated, they can become more difficult to understand and operate, increasing the risk of errors and accidents. In addition, artificial intelligence systems may also malfunction, leading to unexpected results and potential hazards.

Another risk associated with the use of AI in the chemical industry is the possibility of reducing positions and losing jobs for employees. Artificial intelligence systems help automate tasks previously performed by people, which involves the risk of transferring work. In particular, in technologies used by the chemical industry, there are many schematic activities that can easily be automated, leading to significant job losses. However, surveys of employees in chemical companies in Poland indicate a lack of concern about their job security (Kądzielawski, 2022).

In terms of privacy and data security, artificial intelligence systems used in the chemical industry can handle sensitive information and data, such as production processes, chemical formulas, and proprietary information. Ensuring the security and privacy of this data is crucial for protecting a company's intellectual property.

The implementation of artificial intelligence in the chemical industry requires a high level of technical knowledge. Without sufficient specialized knowledge, companies may have difficulty designing, implementing, and maintaining AI systems, leading to suboptimal performance or even failure. Companies that increasingly rely on artificial intelligence systems to optimize their operations may become dependent on the technology. In case of a failure or malfunction of an AI system, companies may not be able to continue their operations, leading to significant financial losses. It is worth noting that with the development of AI systems, there are increasing concerns of ethical nature. For example, AI systems can be used to make decisions that have an impact on human life, such as determining the safety of a chemical product. Without proper supervision and regulation, AI systems can make decisions that are contrary to the interests of society. AI systems rely entirely on data, based on which they are trained. If the data is not sufficiently objective, there is a risk that the AI system will also be biased. Consequently, this situation may lead to unfair decision-making and discrimination.

With the growing integration of AI systems in the chemical industry, there is a risk of cyberattacks. These attacks can disrupt operations, steal confidential information, and cause financial losses.

AI systems in the chemical industry may require integration with other systems, such as enterprise resource planning (ERP) systems, process control systems, and sensor networks. If these systems do not cooperate properly, it may lead to operational inefficiency.

In a study by McKinsey (2019), the implementation phase of AI was divided into 5 stages, and risks were assigned to each of them.

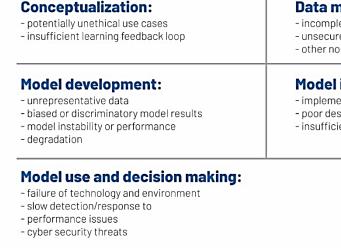


Figure 2. Risks of the 5 stages of AI implementation. Source: own elaboration based on McKinsey, 2019.

Summing up, AI has the potential to revolutionize the chemical industry, but it is important to consider the risks and challenges associated with implementation. These include potential human errors, job loss, data privacy, and security. However, with the proper measures in place, benefits such as increased efficiency, productivity, safety, and sustainable development can be achieved. To maximize benefits and minimize risks, chemical companies should consider a phased approach to AI implementation, starting with pilot projects and gradually increasing scale.

5. Summary

AI technologies have tremendous potential in improving chemical production processes. From demand forecasting to quality control, technologies using artificial intelligence are completely redefining the concepts of chemical production.

Significantly reduced costs, increased production speed, and overall business process efficiency are the new standards that AI tools are introducing. Chemical companies that have already implemented artificial intelligence are showing impressive returns on investment, better product quality, and streamlined supply chain processes.

Effective implementation of new solutions plays a crucial role in the development of chemical industry enterprises. These companies, in order to survive and maintain their market position, will have to change their previously used business models and redefine their value chains. With the planned tightening of environmental regulations and standards in the near future, companies should adapt to current trends - including the circular economy - and utilize digital technology opportunities, as well as enhance the qualifications of their employees in this direction.

Data management :

- incomplete or inaccurate data
- unsecured protected data
- other non-compliances

Model implementation:

- implementation errors
- poor design of technology and environment
- insufficient training and skills building

References

- 1. *5 Pharma companies using artificial intelligence*. Retrieved from: https://www.kantify.com/insights/5-pharma-companies-using-artificial-intelligence, 21.01.2023.
- 2. *A definition of Artificial Intelligence: main capabilities and scientific disciplines*. Retrieved from: https://digital-strategy.ec.europa.eu/en/library/definition-artificial-intelligence-main-capabilities-and-scientific-disciplines, 4.02.2023.
- 3. *Accenture global digital chemicals survey*. Retrieved from: https://www.accenture.com/usen/~/media/accenture/conversion-assets/dotcom/documents/global/pdf/dualpub_6/ accenture-insight-digital-chemical-survey-infographic.pdf, 30.01.2023.
- 4. Andulkar, M., *Dow uses vision AI at the edge to boost employee safety and security with Azure.* Retrieved from: https://customers.microsoft.com/en-us/story/1349423518578860 629 -dow-chemicals-azure-video-analyzer, 16.01.2023.
- Azadeh, A., Bonab, N.A., Salehi, V., Zarrin, M. (2015). A unique algorithm for the assessment and improvement of job satisfaction by resilience engineering: Hazardous labs. *International Journal of Industrial Ergonomics*, 49, 68-77. https://doi.org/10.1016/j.ergon. 2015.06.002.
- Beamon, B.M. (1998). Supply chain design and analysis: Models and methods. *International Journal of Production Economics*, 55(3), 281-294. https://doi.org/10.1016/ S0925-5273(98)00079-6.
- Behdani, B., Lukszo, Z., Srinivasan, R. (2019). Agent-oriented simulation framework for handling disruptions in chemical supply chains. *Computers and Chemical Engineering*, *122*, 306-325. https://doi.org/10.1016/j.compchemeng.2018.0.
- Behdani, B., Lukszo, Z., Adhitya, A., Srinivasan, R. (2009). Agent based model for performance analysis of a global chemical supply chain during normal and abnormal situations. *Computer Aided Chemical Engineering*, 26, 979-984. https://doi.org/10.1016/ S1570-7946(09)70163-4.
- Berning, G., Brandenburg, M., Gürsoy, K., Kussi, J.S., Mehta, V., Tölle, F.J. (2004). Integrating collaborative planning and supply chain optimization for the chemical process industry (I) - Methodology. *Computers and Chemical Engineering*, 28(6-7), 913-927. https://doi.org/10.1016/j.compchemeng.2003.
- Blue Yonder Powers Supply Chain Planning for The Source. Retrieved from: https://media.blueyonder.com/blue-yonder-powers-supply-chain-planning-for-thesource/, 19.01.2023.
- Castillo-Villar, K.K. (2014). Metaheuristic algorithms applied to bioenergy supply chain problems: Theory, review, challenges, and future. *Energies*, 7(11), 7640-7672. https://doi.org/10.3390/en7117640.

- 12. Confronting the risks of artificial intelligence. Retrieved from: https://www.cognitivescale.com/wp-content/uploads/2019/06/Confronting_AI_risks_-___McKinsey.pdf, 16.01.2023.
- 13. Digital transformation initiative chemistry and advanced materials industry. Retrieved from: http://reports.weforum.org/digital-transformation/wp-content/blogs.dir/94/mp/files/ pages/files/dti-chemistry-and-advanced-materials-industry-white-paper.pdf, 30.01.2023.
- Doan, H.A., Agarwal, G., Qian, H., Counihan, M.J., Rodríguez-López, J., Moore, J.S., Assary, R.S. (2020). Quantum chemistry-informed active learning to accelerate the design and discovery of sustainable energy storage materials. *Chemistry of Materials*, 32(15), 6338-6346. https://doi.org/10.1021/acs.chemmater.0c007.
- Ehlen, M.A., Sun, A.C., Pepple, M.A., Eidson, E.D., Jones, B.S. (2014). Chemical supply chain modeling for analysis of homeland security events. *Computers and Chemical Engineering*, 60, 102-111. https://doi.org/10.1016/j.compchemeng.2013.07.
- Ghaderi, H., Pishvaee, M.S., Moini, A. (2016). Biomass supply chain network design: An optimization-oriented review and analysis. *Industrial Crops and Products*, 94, 972-1000. https://doi.org/10.1016/j.indcrop.2016.09.027.
- Gu, G.H., Noh, J., Kim, I., Jung, Y. (2019). Machine learning for renewable energy materials. *Journal of Materials Chemistry A*, 7(29), 17096-17117. https://doi.org/10.1039/ c9ta02356a.
- Guillén, G., Mele, F.D., Espuña, A., Puigjaner, L. (2006). Addressing the design of chemical supply chains under demand uncertainty. *Industrial & Engineering Chemistry Research*, 45, 7566-7581. https://doi.org/10.1021/ie051424a.
- Hájek, P., Stejskal, J. (2018). R&D cooperation and knowledge spillover effects for sustainable business innovation in the chemical industry. *Sustainability*, 10(4), 1064. https://doi.org/10.3390/su10041064.
- Hajjar, Z., Tayyebi, S., Hosein, M., Ahmadi, E. (2016). Application of AI in chemical engineering. In: M.A. Aceves-Fernandez (Ed.), *Artificial intelligence – Emerging trends* and applications (pp. 399-416). https://doi.org/10.5772/intechopen.76027.
- 21. Kądzielawski, G. (2022) The state of development of artificial intelligence in polish industry: opinions of employees. *International Journal of Contemporary Management*, https://doi.org/10.2478/ijcm-2022-0015.
- 22. Komunikat Ministerstwa Rozwoju Pracy i Technologii: Polityka Przemysłowa Polski. Retrieved from: https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd= &ved=2ahUKEwjO7ezMi7X9AhXnhP0HHUPMAYwQFnoECBEQAQ&url=https%3A %2F%2Fwww.gov.pl%2Fattachment%2F555c07a8-4d95-49af-9ec1-282fafdbcac5&usg=AOvVaw1ln80rSkzPhEPBuyvJ0LF7, 16.01.2023.
- 23. Lan, K., Park, S., Yao, Y. (2019). Key issue, challenges, and status quo of models for biofuel supply chain design. In: J. Ren, A. Scipioni, A. Manzardo, H. Liang (Eds.), *Biofuels for*

a more sustainable future: Life cycle sustainability assessment and multi-criteria decision making (pp. 273-315). Elsevier. https://doi.org/10.1016/B978-0-12-815581-3.00010-5.

- 24. Łapińska, J., Kądzielawski, G., Sudolska, A., Górka, J. (2021). Zaufanie pracowników do sztucznej inteligencji w przedsiębiorstwach przemysłu chemicznego. *Przemysł Chemiczny 100(2)*, 127-131.
- Li, Z., Ma, X., Xin, H. (2017). Feature engineering of machine-learning chemisorption models for catalyst design. *Catalysis Today*, 280, 232-238. https://doi.org/10.1016/ j.cattod.2016.04.013.
- 26. Lin, S., Krishnan, V., Womack, D., *Optimizing the chemicals value chain with AI*. Retrieved from: https://www.ibm.com/thought-leadership/institute-business-value/report/chemicals-value-chain-ai, 16.02.2023.
- Marcou, G., Aires De Sousa, J., Latino, D.A.R.S., de Luca, A., Horvath, D., Rietsch, V., Varnek, A. (2015). Expert system for predicting reaction conditions: The Michael reaction case. *Journal of Chemical Information and Modeling*, 55(2), 239-250. https://doi.org/10.1021/ci500698a.
- 28. Matt, Ch., Hess, T., Benlian, A. (2015) Digital Transformation Strategies. *Business & Information Systems Engineering*, 57(5), pp. 339-343.
- 29. Mitsui Chemicals Teams up With NEC and dotData to Trial AI-Based Price Change Forecasting for Market-Sensitive Products. Retrieved from: https://eu.mitsuichemicals.com/release/2021/2021_0924.htm, 19.01.2023.
- Mohammadi, Y., Penlidis, A. (2018). Optimulation in chemical reaction engineering: Oxidative coupling of methane as a case study. *Industrial and Engineering Chemistry Research*, 57(26), 8664-8678. https://doi.org/10.1021/acs.iecr.8b01424.
- OECD (2019). Scoping the OECD AI principles: Deliberations of the Expert Group on Artificial Intelligence at the OECD (AIGO). *OECD Digital Economy Papers, No. 291*. Paris: OECD Publishing, https://doi.org/10.1787/d62f618a-en.
- 32. Pace, R., *Elevating pharma inspection with deep learning*. Retrieved from: https://www.pharmamanufacturing.com/industry-perspectives-sponsored/article/ 11293580/elevating-pharma-inspection-with-deep-learning, 4.02.2023.
- 33. Pozo, C., Ruíz-Femenia, R., Caballero, J., Guillén-Gosálbez, G., Jiménez, L. (2012). On the use of Principal Component Analysis for reducing the number of environmental objectives in multi-objective optimization: Application to the design of chemical supply chains. *Chemical Engineering Science*, 69(1), 146-158. https://doi.org/10.1016/ j.ces.2011.10.018.
- 34. Raport Polskiej Izby Przemysłu Chemicznego pozycja, wyzwania, perspektywy (2022).
- Segler, M.H.S., Preuss, M., Waller, M.P. (2018). Planning chemical syntheses with deep neural networks and symbolic AI. *Nature*, 555(7698), 604-610. https://doi.org/10.1038/ nature25978.

- 36. Smartening up with Artificial Intelligence (AI) What's in it for Germany and its Industrial Sector? Retrieved from: https://www.mckinsey.com/~/media/mckinsey/industries/ semiconductors/our%20insights/smartening%20up%20with%20artificial%20intelligence/ smartening-up-with-artificial-intelligence.ashx, 30.01.2023.
- Specialty Chemicals Market Size, Share & Trends Analysis Report By Product (Institutional & Industrial Cleaners, Flavor & Fragrances, Food & Feed Additives), By Region, And Segment Forecasts, 2023-2030. Retrieved from: https://www.grandviewresearch.com/ industry-analysis/specialty-chemicals-market, 2.02.2023.
- Vinuesa, R., Azizpour, H., Leite, I. et al. (2020). The role of artificial intelligence in achieving the Sustainable Development Goals. *Nat Commun*, *11*, 233. https://doi.org/10.1038/s41467-019-14108-y.
- Zahrt, A.F., Henle, J.J., Rose, B.T., Wang, Y., Darrow, W.T., Denmark, S.E. (2019). Prediction of higher-selectivity catalysts by computer-driven workflow and machine learning. *Science*, 363(6424), 1-11. https://doi.org/10.1126/science.aau5631.
- Zhao, K., Yu, X. (2011). A case based reasoning approach on supplier selection in petroleum enterprises. *Expert Systems with Applications*, 38(6), 6839-6847. https://doi.org/10.1016/j.eswa.2010.12.055.
- Zhou, Z., Li, X., Zare, R.N. (2017). Optimizing chemical reactions with deep reinforcement learning. ACS Central Science, 3(12), 1337-1344. https://doi.org/10.1021/acscentsci. 7b00492.