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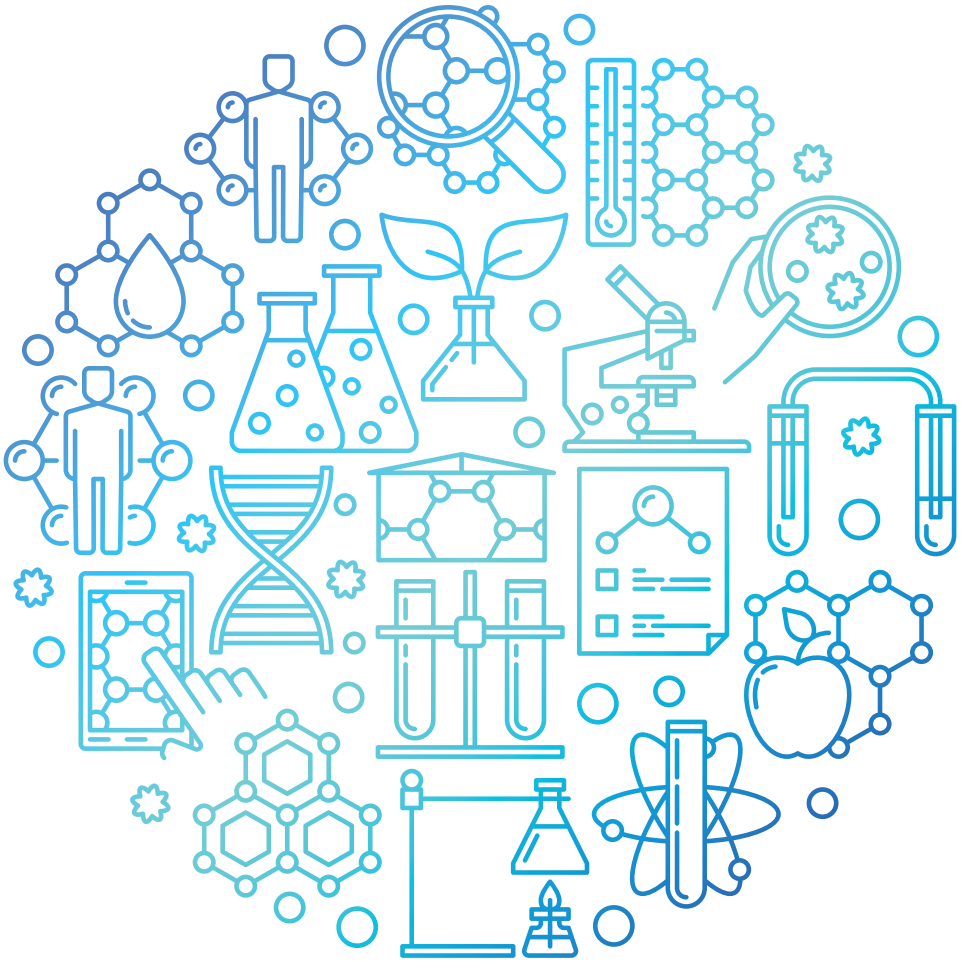


Chemicals Insights

Shaping tomorrow's innovations through AI

In our summer 2024 Chemicals Insights, we explore the transformative potential of AI in the chemical industry's R&D processes, the growing significance of ESG provisions in sales and purchase agreements, and the evolving market dynamics reflected in economic forecasts. Our latest edition aims to unpack these complexities as the industry embraces change.

MAKING AN IMPACT THAT MATTERS since 1845

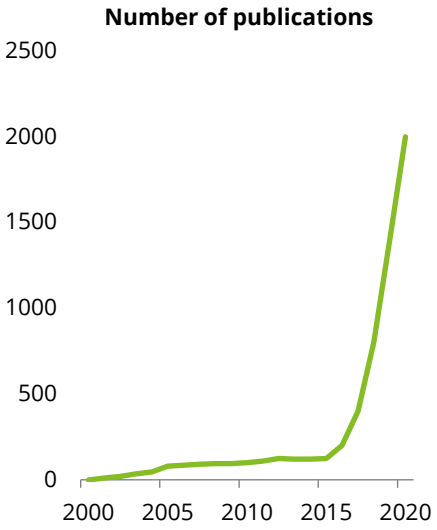
Hot topics in the market – Unleashing the power of AI in chemistry

In the rapidly developing digital world, there is no doubt that artificial intelligence is the talk of the day. At the same time, the chemical industry is facing more challenges than ever, including increased international competition (particularly when it comes to securing investments) and mounting sustainability requirements impacting products, processes and applications alike. What all these forces have in common is that they are intensifying the call for innovation and efficiency throughout the chemical industry's value chain.

Therefore digitalization, quantum computing and artificial intelligence (AI) are not only technological advancements in the chemical industry, but also key drivers to successfully managing the upcoming challenges and paving the way for smarter, more efficient and sustainable processes.

Chemical companies have recognized the necessity of implementing artificial intelligence, as evidenced by the trend in patent publications (see Figure 1).

Fig. 1 – Annual publication volume of AI-related chemistry patents from 2000-2020



Source: CAS, American Chemical Society 2021, Artificial Intelligence in Chemistry.

While digitalization transforms analog processes into digital ones, quantum computing offers unparalleled computational capabilities. AI, with its algorithms and machine learning process, revolutionizes decision-making and process optimization.

Another indicator are chemistry-related AI publications. The United States and China have been leading the charge for the past five years, with a combined total of more than 40% of global journal contributions. Meanwhile, another 20% share comes from India, Iran, the UK, and Germany combined.

Integration of AI into chemicals R&D

In research and development, AI can, for example, facilitate the design of new molecules. Through complex calculations and prediction models, AI systems can analyze and optimize potential molecular structures to achieve the desired chemical properties. As an example, one of the largest chemical companies globally is leveraging a supercomputer for tasks such as calculating the most promising polymer structure from thousands of possibilities. With a staggering capacity of 3 quadrillion floating-point operations per second, this supercomputer boasts computing power equivalent to approximately 20,000 laptops.

But it is not just about computer power. It is important to automate data filtering and analysis, with tools such as AI, ML (machine learning), and data mining. Data visualization techniques can aid in the presentation of data, making it easier to comprehend and identify trends. [1, 2, 3]

But AI can do even more by linking automated R&D with production. Scientists at Carnegie Mellon University in Pittsburgh have developed an AI system that not only designs chemical experiments, but also carries them out autonomously. This artificial intelligence controls a robotic laboratory that fully automates the various chemical processes. In initial tests, the AI independently conducted research and planned the production of pharmaceuticals such as ibuprofen. In doing so, it coordinated a complex sequence of catalysis reactions, all without any human involvement. [4]

Process optimization

Given the huge variety and complexity of process parameters, physical and chemical processes, and substances involved, process optimization is a key area for value creation.

Here, AI can predict under which conditions the best yields can be achieved or the fewest by-products formed. Lapkin et al. developed a novel hybrid mechanistic machine learning approach for solvent selection, identifying promising solvents for asymmetric hydrogenation, outperforming human intuition in terms of conversion and diastereomeric excess. By emphasizing screening charge density as a solvent descriptor and using a dimensionality-reduced set of physiochemical descriptors, models

1 Chen et al., Temperature swing adsorption for CO2 capture: Thermal design and management on adsorption bed with single-tube/three-tube internal heat exchanger, 2021, accessed 28 May 2024.
2 Chen et al., The mutual benefits of renewables and carbon capture: Achieved by an artificial intelligent scheduling strategy, 2021, accessed 28 May 2024.
3 Helei et al., Technology development and applications of artificial intelligence for post-combustion carbon. dioxide capture: Critical literature review and perspectives, 2021, accessed 28 May 2024.
4 Royal Society of Chemistry, First GPT-4-powered AI lab assistant independently directs key organic reactions | Research | Chemistry World, 2024, press release 08 January 2024.

suggested more than 15 solvents achieving greater than >90% conversion, compared to one solvent suggested by a human expert. [5]

AI-powered process optimization also supports the achievement of sustainability targets. In particular carbon capture, utilization and storage (CCUS) is a key area of AI application. By analyzing vast amounts of data in real time, AI algorithms optimize CO2 capture systems, leading to cost reduction and increased efficiency. Additionally, AI improves system accuracy and reliability by making real-time adjustments, preventing breakdowns and ensuring long-term operational efficiency.

There are also other areas besides CO2 capturing where AI can make a difference, including the development of more efficient catalysts for chemical reactions. Szekely et al. extend the application of AI to develop materials in an environmentally friendly way. They demonstrate successful materials development by combining the design of experiments with a new machine learning module that comprises a support vector machine, an evolutionary algorithm, and a desirability function. They use their AI-based method to realize the sustainable electrochemical synthesis of a ZIF-8 metal-organic framework. The incorporation of an evolutionary algorithm (NSGA-II) enabled a rapid and accurate methodology to obtain ZIF-8 with 100% purity, 88% yield, and 86% crystallinity. The E factor, energy consumption and carbon footprint were minimized to 11 kg kg−1, 7 kW h kg−1 and 27 kg kg−1, respectively. [6]

Supply chain optimization

In supply chain optimization, AI enables more accurate forecasting of demand and delivery times, leading to more efficient inventory and logistics processes. In addition, it enables automated quality control by detecting quality deviations in real time and suggesting or implementing corrective actions. This helps to consistently maintain product quality at a high level and minimizes defect rates. Moreover, artificial intelligence supports preventive maintenance planning through the analysis of operational data. In concrete cases, AI has been able to reduce forecasting error by 50% compared to human forecasting. [7]

Value creation to the end customer

But process efficiency is not the only aspect. AI in the chemical industry can help to generate value for the end customer as well, such as by providing support in product formulation in the paints and coatings industry. It helps to identify optimal mixing ratios to achieve the desired product properties. A leading global coatings manufacturer utilizes AI-powered natural language systems to understand descriptions of the ideal color. Users begin with a general description, such as "New York City summer sunset," and then refine their preferences based on the system's responses. These responses may include photos and additional options, allowing users to make more detailed adjustments like choosing a darker red, adding moodiness, or incorporating a touch of sunlight until they achieve the desired color. [8]

Outlook

Overall, the integration of AI into the chemical industry offers significant potential for driving innovation, enhancing efficiency, quality, and sustainability by optimizing production processes as well as reducing time and resource consumption. The combination of advanced technology and ecological thinking not only leads to economic value but also contributes to the sustainability goals of the chemical industry. [9]

However, there are also risks and challenges to consider. These include concerns about data privacy and security, the risk of wrong decisions by AI systems, and a potential dependence on technology, as well as ethical issues such as bias in algorithms. Furthermore, processing and interpreting complex chemical data require advanced AI models and interdisciplinary collaboration between chemists, engineers, and IT experts. Compliance with regulatory requirements, continuous technological advancements, and the high investment costs associated with implementing AI systems are also significant challenges.

Would you like to learn more about how AI is shaping the future of research and development in the chemical industry? Take a look at our latest Energy & Chemicals Industry Insights: 'Next Generation R&D'. Dive in and discover how AI and other innovative technologies are shaping the future of our industry. Stay informed and inspired with Deloitte.

5 Amar et al., Machine learning and molecular descriptors enable rational solvent selection in asymmetric catalysis, 2019.
6 Hardian et al., Artificial intelligence: the silver bullet for sustainable materials development, 2020.
7 Postindustrial, AI in Chemical Industry: Use Cases, Benefits, and Challenges, 2022, accessed 28 May 2024.
8 Fast Company, This new AI-powered paint tool helps you create custom colors with your voice - Fast Company, 2022, accessed 28 May 2024.
9 Yaqub et al., Process optimization of chemical looping combustion of solid waste/biomass using machine learning algorithm, 2024, accessed 28 May 2024.

Sustainability update – ESG related clauses in SPAs and post-M&A disputes

It is impossible to imagine the future of M&A transactions without assessing ESG opportunities and risks. However, the increasing number of ESG disputes shows that the associated risks are still being underestimated.

While ESG factors in due diligence are becoming part of the standard repertoire, sellers and buyers still face considerable challenges when integrating sustainability aspects into their transaction documents, including the sale and purchase agreement (SPA). These issues are displayed in Figure 2, on the right of the page.

Despite these difficulties, efforts to incorporate ESG factors into the SPA are worthwhile, both from a legal and a financial perspective. ESG aspects can play an important role in the calculation and negotiation of the purchase price and are regularly part of cost- and time-intensive post-M&A disputes. Moreover, sellers can shield themselves from future ESG-related indemnification payments, while buyers can actively protect themselves against potential ESG risks.

Pilot initiatives

To support the green transition and meet the challenges of the actors involved, some pilot initiatives have drafted ESG-specific SPA clauses. The Chancery Lane Project (TCLP) is a global association of 3,600 lawyers and business leaders, as well as 375 organizations from 113 countries, that aim to drive global decarbonization with the help of climate contracting. Its website offers free access and usage rights to more than 100 topic- and industry-specific, peer-reviewed climate clauses and more than 70 climate-related glossary terms, drafted and assessed by industry and legal experts.

The second initiative is the Working Group Model Contract Clauses 2.0 (MCCs 2.0) launched by the American Bar Association's Business Law Section. With a focus on US state law and the United Nations Convention on Contracts for the International Sale of Goods, this group has set itself the task of translating the UN Guiding Principles on Business and Human Rights (UNGPs) and the OECD Due Diligence Guidance for Responsible Business Conduct (OECD Guidance) into contractual obligations so that business actors can include them in supply contracts for the manufacture and sale of goods. The standard clauses of both projects offer industry-specific guidance and a basis for drafting transaction-specific clauses.

Current ESG clauses in SPAs

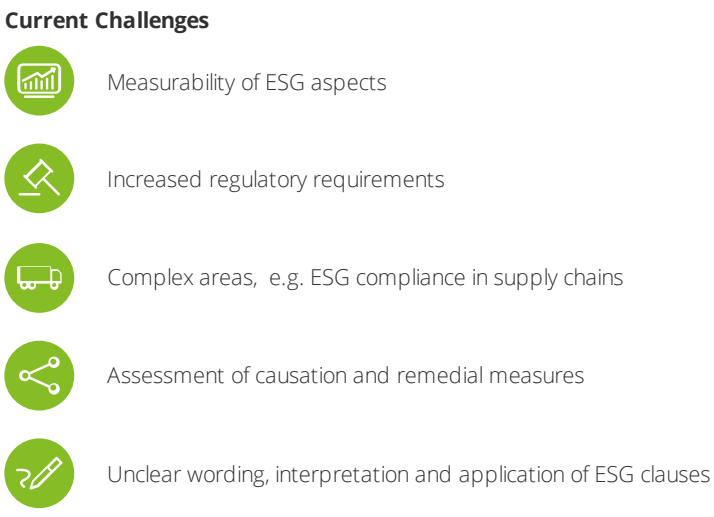
Environmental clauses that refer to compliance with existing environmental protection laws are already standard in SPAs. Typical examples of more current ESG-specific contractual clauses include climate change/net-zero targets, human rights and/or anti-discrimination obligations, and renewable energy commitments. ESG-specific clauses can be included in different parts of the SPA to meet the interests of both seller and buyer. This includes ESG legal aspects in representations, warranties, and indemnities. Beyond the assurance of there being no evidence of climate-related litigation, a popular example of representations and warranties in the US context is the "Weinstein clause", which arose from the #MeToo movement, and compels companies to disclose allegations of sexual harassment. ESG-related contractual agreements furthermore offer buyers the opportunity to protect themselves against cases of greenwashing that were not identified during due diligence.

ESG risk management in contracts

Analysis of ESG-related liabilities and reputational risks is the basis for their inclusion in the contract documents. Under indemnity agreements, buyers can protect themselves against sustainability risk identified during due diligence but unclear at the time of signing in terms of outcome or associated costs, for instance a pending investigation into specific environmental pollution and the costs associated with its remediation. For effective dispute prevention, the wording of such agreements should be as specific as possible. Current post-M&A disputes reveal the added value that consideration of ESG aspects in transactions would bring. Disputed items that are regularly dealt with include provisions for environmental protection obligations, CapEx investment obligations required by extended ESG regulation, and use-based accounting of CO2 certificates. SPAs that consider ESG risks and opportunities function as a valuable tool for dispute prevention, helping sellers and buyers avoid the time and costs spent on later ESG disputes.

You can find more updates on the latest ESG developments on Deloitte's ESG Blog: Integrating ESG in M&A | Deloitte Germany

Fig. 2 – Challenges for the integration of sustainability aspects into transaction documents



Economy updates – Cautiously optimistic developments

Eurozone economies have had a mixed start to 2024. The good news is that inflation has been easing faster than economists had initially expected, and labor markets are still surprisingly robust; but the bad news is that there are still no clear signs of an upturn in household spending – the key driver of the 2024 outlook – leaving an economic recovery somewhat postponed. Altogether, we can expect a year of moderate growth with gradually increasing economic activity.

Fragile and divergent economic situation

Economic growth (in terms of gross domestic product) in the eurozone slowed from an annual pace of 3.4% in 2022 to 0.4% in 2023. The slowdown was more pronounced in the second half of the year, with GDP contracting slightly in the third quarter before stagnating in the fourth. A combination of factors drove this weakness. Annual figures show that consumer expenditure expanded only slightly, as consumers were reluctant to spend more in the face of still-high inflation and increased savings due to high interest rates and economic uncertainty. However, the robust labor market prevented a greater slowdown.

Investment activity also lost momentum as elevated financing costs and uncertainty made many investment projects appear less attractive. Furthermore, subdued foreign demand caused the eurozone's export levels to contract; but the trade balance remained positive overall as imports contracted even more in comparative terms.

Yet these developments were not spread uniformly across sectors or countries. Looking at economic activity (measured by value added) by sector, manufacturing contracted in 2023 and construction grew only slightly, marking a slowdown from prior years. Economic activity slowed in services as well, but to a lesser extent since the sector is generally less prone to increases in energy prices and financing costs, given that it is less energy- and capital-intensive. In particular, information and communications, as well as sectors including entertainment, recreation, and other services, were still able to expand with healthy growth rates.

In terms of countries, Germany was the poorest performing of the major eurozone nations, with its GDP contracting slightly by -0.3% in 2023 compared to the previous year. The decline of German economic activity was broad-based, but energy-intensive and energy production-related industrial sectors struggled in particular. On the other hand, the Spanish economy grew by 2.5% resulting from continuing tourism growth and benefiting particularly from increasing international tourism. Between these two extremes lie the moderately growing economies of Italy and France.

Despite easing inflation and a strong labor market, consumers in the eurozone are still holding back on spending.

Inflation and private consumption to determine recovery pace

Lately, inflation has been easing faster than expected, with the European Central Bank revising its inflation forecasts downward in early March.[10] However, services inflation has been stagnant between 3.7% and 4% since November 2023,[11] mainly because wage growth is still strong and softening only slowly. This plays a crucial role for services inflation as the sector is labor-intensive.

Easing inflation (and thus, higher real income) has slowly been reflected in the willingness to make purchases. Retail sales increased in March[12]; consumer sentiment is also picking up[13]; and savings intentions remain elevated among consumers.[14] These factors point to a possible postponement of the recovery of household expenditures until later in the year. On the other hand, the recovery might be slightly stronger if part of these savings will be used later (as interest rates come down and uncertainty fades) for consumption to fulfill pent-up demand.

Sectoral differences to continue

The outlook for businesses varies across sectors. The situation in manufacturing seems to remain difficult as indicated by the HCOB Manufacturing Purchasing Managers' Index, which did not follow the upward trend of the previous months but plateaued in February and March and is still in contractionary territory.*

While index values for German manufacturing are barely moving upward, other major eurozone economies seem to be recovering much more quickly. The industrial confidence of the European Commission stands well below its long-term average, with no clear direction. Altogether, the manufacturing sector is unlikely to deteriorate further; the pace of decline seems to be softening despite a quick rebound being more or less unlikely.

Outlook

We expect a consumption-driven recovery to start slowly over the course of 2024 as disinflation continues, nominal wages increase, and thus real incomes continue to rise. Investment activity should start to pick up later as financing conditions start to ease and economic uncertainty diminishes. Overall, economic activity in the Eurozone should increase with GDP growing by 0.6% in 2024 and 1.6% next year. We expect inflation to decrease to an annual rate of 2.3% in 2024 and 1.9% in 2025.

Regular economic updates are provided in our Deloitte Insights: Economics: EMEA | Deloitte Insights.

* Index readings higher than 50 indicate an economic expansion, and readings below 50 indicate an economic contraction.

10 European Central Bank, ECB staff macroeconomic projections for the euro area, accessed 28 May 2024.
11 Eurostat, Annual inflation stable at 2.4% in the euro area, 17 May 2024.
12 Eurostat, Volume of retail trade up by 0.8% in the euro area and by 1.2% in the EU, 07 May 2024.
13 European Commission, Latest business and consumer surveys, May 2024, accessed 28 May 2024.
14 Eurostat, Consumers – monthly data, accessed 28 May 2024.

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